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SPILL ASSESSMENT MODEL USER'S MANUAL.(U)
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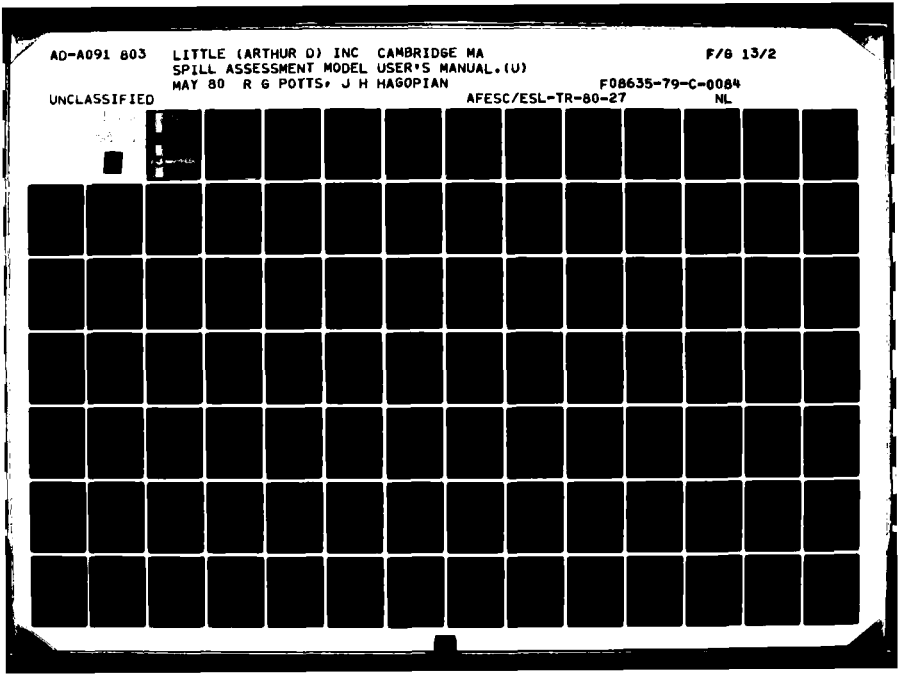

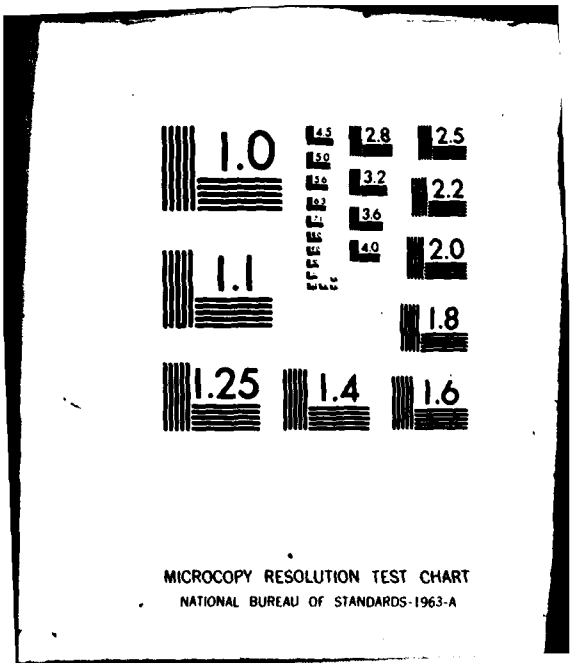
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SPILL ASSESSMENT MODEL USER'S MANUAL

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MAY 1980

FINAL REPORT
FEBRUARY 1979 – FEBRUARY 1980

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

(19) REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER ESL-TR-80-27 ✓	2. GOVT ACCESSION NO. AD-A091 803	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) (6) SPILL ASSESSMENT MODEL USER'S MANUAL		5. TYPE OF REPORT & PERIOD COVERED (9) FINAL REPORT, FEB[illegible]1979-FEB[illegible]1980, 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) (10) RICHARD C. POTTS JOHN H. HAGOPIAN		8. CONTRACT OR GRANT NUMBER(s) (15) F08635-79-C-0084 ✓
9. PERFORMING ORGANIZATION NAME AND ADDRESS ARTHUR D. LITTLE, INC. ✓ ACORN PARK CAMBRIDGE, MASSACHUSETTS 02140		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS (16) JON: SAMS-DP-02 (17) DP PE: 78001F
11. CONTROLLING OFFICE NAME AND ADDRESS (11) AIR FORCE ENGINEERING AND SERVICES CENTER TYNDALL AIR FORCE BASE, FLORIDA 32403		12. REPORT DATE MAY 1980 13. NUMBER OF PAGES (12) 184 182
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

AVAILABILITY OF THIS REPORT IS SPECIFIED ON VERSO OF FRONT COVER.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

HYDRAZINE, SPILL, HAZARDOUS MATERIALS, WATERWAYS, RIVERS, LAKES, ESTUARIES, CHEMICAL DECAY, DISPERSION, MODEL, INTERACTIVE, COMPUTER

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

THIS REPORT IS A USER'S GUIDE TO THE SPILL ASSESSMENT MODEL (SAM) WHICH IS A MATHEMATICAL MODEL FOR APPLICATION IN ASSESSING THE IMPACT OF CATASTROPHIC SPILLS IN WATERWAYS AS DEVELOPED IN ESL-TR-80-07. THE SPILL MODEL ADDRESSES INSTANTANEOUS AND CONTINUOUS POINT SOURCE DISCHARGES INTO WATER COURSES INCLUDING RIVERS, LAKES, STREAMS, AND ESTUARIES. THE MODEL IS IN A GENERALIZED FORM USING PARAMETERS AND INTERCHANGEABLE DATA ITEMS SO AS NOT

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20. ABSTRACT (CONCLUDED)

TO UNNECESSARILY RESTRICT THE SCOPE OF APPLICATION TO HYDRAZINE. SAM ESTIMATES THE EXTENT AND DURATION OF HAZARDOUS CONCENTRATIONS IN WATER-BODIES ASSOCIATED WITH ACCIDENTAL DISCHARGES AND DETERMINES WHEN THESE CONCENTRATIONS DROP BELOW TOXIC LEVELS. SAM IS DESIGNED AS A MANAGEMENT TOOL TO SUPPORT CLEAN-UP OPERATIONS IN THE EVENT OF A SPILL, TO PERMIT POST-INCIDENT ANALYSES, AND TO SERVE AS A BASIS FOR CONTINGENCY PLANNING.

SAM IS BASED ON PREVIOUS DEVELOPMENT FOR THE U.S. COAST GUARD IN THE DESIGN, DEVELOPMENT, AND IMPLEMENTATION OF THE HAZARD ASSESSMENT COMPUTER SYSTEM (HACS).

PREFACE

This report was prepared by Arthur D. Little, Inc., Acorn Park, Cambridge, Massachusetts 02140 under Contract No. F08635-79-C-0084 with the Air Force Engineering and Services Center, Tyndall Air Force Base, Florida 32403. The work was begun in February 1979 and was completed in February 1980.

This report has been reviewed by the Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS). At NTIS it will be available to the general public, including foreign nationals.

This technical report has been reviewed and is approved for publication.

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INTRODUCTION

Current U.S. Air Force operations dictate the use of numerous toxic substances, and among these are the three hydrazine family fuels (anhydrous, unsymmetrical dimethyl, and monomethyl hydrazine). Hydrazine fuels are the basic rocket propellant for strategic missiles and satellites, and the joint NASA and USAF sponsored Space Shuttle Program will greatly increase the volume of hydrazine in general use. Bulk storage and transport of hydrazine fuels could lead to accidental discharges, and if a discharge finds it way into a water body, undesirable consequences could occur to the aquatic ecosystem.

This report is a user's guide to a computerized spill model called the Spill Assessment Model (SAM) which is available to obtain estimates of the concentration in water resulting from a spill or accidental discharge of a hydrazine family fuel or other materials which are soluble in water. The Spill Assessment Model has been based on previous development for the U.S. Coast Guard in the design and implementation of the Hazard Assessment Computer System (HACS). SAM has been implemented within the framework of HACS, together with an interactive terminal interface. This manual contains sufficient information to operate the water dispersion model. However, if the full capabilities of the HACS system are required, users should refer to U.S. Coast Guard publications for complete instructions regarding other models in the system. A complete description of the formulation of the water dispersion model is available in a separate technical report, ESL-TR-80-07, and a field manual, ESL-TR-80-22, for

non-computerized use of the model.

The spill model addresses instantaneous and continuous point source discharges into water courses including rivers, lakes, streams and estuaries. The primary requirement of the model is to assess dispersive characteristics of spills of the hydrazine family fuels in the aquatic environment, however, the implementation of the model within the HACS framework has permitted a generalized form using parameters and interchangeable data items so as to not unnecessarily restrict the scope of application. Results which can be produced by the model include the pollutant concentration as a function of location, time, and physical, chemical and biological characteristics of the pollutant. A spill model of this type estimates the extent and duration of hazardous concentrations in water bodies associated with accidental discharges, and when these concentrations drop below specified toxic levels. Such a model could become a management tool to support emergency responses or clean-up operations in the event of a spill, to provide for emergency discharge contingency planning, permit post incident analyses, and serve as a basis for further development of methods of hazard assessment.

The spill model computes the concentration of a water-miscible liquid or solid at any specified point and given time for a discharge on the surface of a lake, river, or estuary. All the chemical discharged is assumed to go into solution with water. The same model can also be used for the dispersion of insoluble solids which are neutrally buoyant or whose settling times are large compared to mixing times. The model can also be used approximately for concentration estimates

for those liquids which react with water or whose boiling point is less than that of ambient temperature.

The computer model described in this manual is written in Fortran IV, and operates on CDC 6600 computers under the NOS operating system to interface with an interactive remote terminal for input/output. Four disk storage files are used: source program storage, object code storage, external file of chemical property data, and default file containing nominal values for model data items. Approximately 68K words of memory are required during execution of the complete model.

Section II of this manual presents a framework for hazard assessment, mainly derived from the CHRIS system of the U.S. Coast Guard, to describe the context within which the spill model may be utilized, and Section III gives a summary overview of the operating concepts of the spill model within HACS.

Section IV defines the types of water bodies currently modeled, introduces the system of spatial coordinates, describes the types of chemical discharges which are modeled, and includes additional discussion of modeling chemical degradation after discharge.

Specific instructions for the operation of the spill model are given in Sections V and VI with illustrative system prompts, descriptions and tables of data items with explanations. Three sample problems are given in Section VII and provide further illustration of the use of the spill model. Section VIII gives a review of the significant assumptions incorporated in the formulation of the spill model. Appendices contain tables of chemical specific codes and synonyms, explanations of additional system messages, and definitions of data item unit labels.

SECTION II

FRAMEWORK FOR HAZARD ASSESSMENT

SAM has been implemented from the framework of the Hazard Assessment Computer System (HACS). HACS itself was originally developed as a component of the Chemical Hazard Response Information System (CHRIS) under the sponsorship of the U.S. Coast Guard. Both CHRIS and HACS provide a systematic, simplified approach to identifying the appropriate processes governing a given chemical release and methods for estimating the hazard. Basic hazard estimates can be obtained in terms of distances over which a toxic or flammable concentration of a given chemical may exist and the minimum safe distance between the spill site and people, combustible materials or protected resources, should the chemical ignite and a fire ensue.

One of the spill models originally formulated for use within HACS and CHRIS addressed the prediction of hazards caused by the accidental spill of a toxic chemical miscible with water, on different types of receiving water bodies. When a miscible chemical is spilled on the water surface, it rapidly mixes with the water. This mixing is primarily caused by flow non-uniformities (turbulence) or in some cases by wave action. Because of the predominance of certain types of phenomena in different regions of the different types of receiving water bodies, the model for water dispersion of miscible substances is actually composed of a series of different theoretical predictive methods, for the purpose of estimating the concentration levels of the dispersing chemical in water at different locations and different times after the occurrence

of a spill at some point.

Since the model described in this manual addresses only the dispersion of miscible substances in water, it is important to recognize and emphasize that the model describes a particular type of chemical behavior, and the consequences of that behavior. Additional hazards may result from other behavior on release; therefore, in this section the overall framework for hazard assessment provided by CHRIS and HACS is introduced and the approach and concepts employed in these systems are briefly described.

1. OVERVIEW

CHRIS and HACS are designed to enable quick and accurate estimates of hazards presented by a discharge, or potential discharge, of hazardous chemicals, and to provide these estimates in a form useful to response personnel. The broader scope of CHRIS encompasses a compendium of chemical data, data on response methods, data bases for contingency plans, and field manuals, in addition to analytical methods and manual procedures for quickly obtaining hazard estimates. HACS was originally developed as an extension of the analytical procedures included in CHRIS, for manual field assessment of potential hazards, to extend the level of detail and accuracy beyond that possible for simplified field procedures.

HACS is a computer-based system, incorporating the mathematical models originally developed as the basis for the field calculation procedures implemented in CHRIS, and a number of specialized models developed specifically for computer applications. The design and

implementation of HACS focused on providing rapid and quantitative assessments in response to questions such as the following:

- When will the air/water concentration of discharged material reach a specified level of toxicity at a given location?
- When will the air/water concentration return to a specified safe or nontoxic level?
- What is the concentration of discharged material at a specified location and time?

Both CHRIS and HACS are generalized systems, encompassing different types of chemical behavior and different types of hazards. They have been designed for use under emergency conditions involving the actual or potential accidental discharge of a hazardous material into navigable waters and for such non-emergency uses as contingency planning (pre-planned assessments and responses), training, and evaluation and improvement of assessment methods.

2. INFORMATION AND USE REQUIREMENTS

The evaluation of a hazard due to a chemical discharge was considered to involve the following sequence of action:

- Determination of information pertinent to the on-scene conditions at the spill site.
- Selection of appropriate calculation procedures.
- Evaluation of the extent of hazards as indicated by these calculations.

The types of information relating to the discharge conditions at the scene of the spill are:

- Discharged chemical characteristics (e.g., name, temperature, quantity).
- Discharge conditions (e.g., tank size, location of discharge opening relative to water's surface).
- Environmental conditions (e.g., wind speed, air and water temperatures).
- Marine conditions (e.g., current speed, water depth at spill site).

3. SPECIFICATION OF SPILLED MATERIAL AND MODEL CODE

Once the identity of the discharged chemical and the associated hazard assessment code have been established as can be determined in Appendices A and B, the appropriate hazard assessment calculation procedures can be carried out. In SAM the calculation procedures are embodied in a set of specific computer programs for estimating discharge conditions and chemical behavior. Each program contains one or more mathematical models for the calculation procedures, and the individual models contained within SAM are also identified by similar one or two letter codes. In the present configuration, those models applicable to discharges of the hydrazine fuels include: (A) release or discharge model; (P) concentration of water-miscible liquid or solid for a discharge into a lake, river or estuary; (Q) pool fire model for soluble liquids which have a boiling point greater than ambient; (R) for vapor evolution from a chemical discharge into water; and (S) for vapor dispersion in support of model R. The work described in this manual addresses the refinement and enhancement of the model for the concentration of

a miscible chemical in water (P).

SAM provides estimates of hazards in the following manner. The system first begins by accepting user input which provides identification of the chemical substance which was spilled, discharge conditions, marine conditions, environmental conditions, etc.

To obtain detailed chemical specific properties, the current models automatically interface with a separate data base containing information on 900 chemicals. Each chemical is identified by a 3 letter code which is entered by the user to retrieve the desired physical property data. The codes for the hydrazine fuels are: DMH (unsymmetrical dimethyl hydrazine); HDZ (hydrazine); and MHZ (methylhydrazine). Physical properties for these chemicals are recorded as data constants or empirical functions of temperature.

4. SELECTION OF ADDITIONAL INPUT DATA

Some properties, not measured in the laboratory, have been estimated using techniques which have been proven acceptably valid for similar chemicals. The techniques were selected and utilized by R. Reid, co-author of the standard reference, "The Properties of Gases and Liquids" by Sherwood and Reid. Properties are arranged in alphabetical order by chemical code (the three-letter recognition code assigned to each chemical), and all properties pertaining to a given chemical are contained in one logical record, automatically available to SAM for conducting a hazard assessment.

Since not all items used in the file apply to each chemical, a data quality or type scheme is used. Each data item in the file, for

each chemical, has a code assigned with it to indicate whether the value entered is exact, an estimate, or not applicable. The properties for a given chemical are accessed by specifying the recognition code for the desired chemical. This is the only input required by the user to obtain the required physical and chemical properties associated with the discharged chemical. However, the data type scheme provides a means for allowing data entered by the user to override values that would otherwise be selected from the property file. Thus, more accurate chemical data, if available, can readily be substituted, or the effects of variations in physical properties can be investigated.

If SAM requires additional data that has not been provided by the user or obtained from the chemical properties file, the system automatically retrieves nominal values from an internal default file. The default file is used to (a) define the characteristics and units of measure of all input items and computed results and (b) provide reasonable estimates or default values for each item to enable hazard assessments to be made under conditions of limited data availability.

5. CONTROLS

Overall control of the input operations is provided by the user input processor which accepts and stores user input data in optional systems of measure, provides limit tests for the reasonability of input data and estimated computed hazard levels, coordinates the internal use of data and computed values according to a data item quality hierarchy, and provides overall control of the assessment computation sequence (for example, allowing single runs, or iterative computations for

sensitivity analyses). This portion of the system also contains all generalized software used for producing output reports and plotted displays of model outputs. On completion of the input processing step, SAM begins the estimation or assessment calculations.

6. OUTPUT

When the execution of the models specified for a particular hazard assessment scenario has been completed, the system produces textual reports, and, if desired, optional tables and/or plotted output displays. The system output identifies the spilled chemical, restates the discharge, environmental and marine conditions and reports the hazard assessment. The output information provided enables the user to validate input data quickly and accurately. The system can plot concentration as a function of location and/or time. The objective of the system is to obtain and display estimates of the dispersion of a chemical or the effects of that dispersion in the environment as a function of distance and time in terms of the extent to which toxic limits may be exceeded. The subjective interpretation of the potential hazards as a consequence is not included within the scope of the system.

SECTION III

CONCEPTS AND STRUCTURE OF SAM

This section provides an overview of the different program components, data files, and sequences of operation. Concepts of the SAM data structure and manipulation are presented in some detail to aid in understanding the operation of the spill model and its interaction with the other components of the system.

1. SAM COMPONENTS

SAM consists of several program components:

- Executive System -- to control the overall sequence of operations, and to provide utility functions for data base input/output operations, line printer or remote terminal plotting, output labeling and program overlay and segment loading.
- User Input Processor -- to read, verify, and store user input data and to control the initialization of SAM data files.
- Property Data Processor -- to retrieve requested data from the property file, perform unit conversions to internal CGS units, to compute values of functions of temperature, and to transfer chemical specific property data to the state file.
- Assessment Models -- a series of separate programs retrieving required data from the state file, performing the indicated assessment computations, storing computed values in the state file for subsequent use, and generating specified plotted and tabulated output.

These components utilize a number of both internal and external files in their operations. These files include:

- Program File -- a permanent disk file containing pre-compiled program code in overlay and segment structure. The executive system automatically accesses this file to load portions of the program code into computer memory for execution as required.
- State File -- an internal program file constructed by SAM during an assessment run; provides data base storage for all user input, property, default and computed data items utilizing a data quality priority structure.
- Default File -- a permanent disk file defining the structure of the SAM state file and containing estimated values for data items to be used only in the absence of any other value.
- Chemical Properties File -- an external file containing predefined physical property data for 900 hazardous chemical substances.
- Save File -- an internal program file containing a copy of a state file after completion of initialization operations. Permits re-runs requiring only new input values to be used.

a. State File

The state file contains all information necessary for the operation of SAM. It provides storage for all input variables for the execution

of models and output information (units, values, print names, etc.) for all computed results.

At the start of each new run, the contents of the state file are initially obtained from the default file. This provides basic definitions of each data item (see below) and default values which are only used in the event that no other value is supplied or obtained. The input variables for the execution of models are then obtained by the User Input Processor from the user terminal, and the Property Data Processor from the chemical properties file, and stored in the state file. When a model is executed, the information necessary for the execution of that model is retrieved from the state file, and the results of a model's execution are then stored back into this file. Thus, when another model is to be executed, it has access to input information and the computed results of a previously executed model. For each variable in the state file, the information stored includes:

- Variable number -- a unique four digit number (such as 2015) identifying the input or output quantity; also referred to as field number.
- Type of quantity -- an indicator referencing the permitted units in which values of the variable may be entered, and the conversion factors used to obtain values stored in the state file in CGS units for internal operations.
- A source or priority code -- to indicate the origin of the data item stored in the state file. These priority codes are as follows:

0 - No value present

1 - Default file value

2 - Chemical property file estimate

3 - Chemical property file exact value

4 - Computed value

5 - User supplied data value

6 - System value

For a value of a variable to be used in place of an already existing value of the same variable, it must have a source or priority code that is numerically higher than the source code of the existing value.

- The value of the input quantity or calculated result.
- The nominal minimum value that the variable is reasonably expected to reach.
- The nominal maximum value that the variable is reasonably expected to attain.
- The display name of the variable for identification of the variable in output reports.

As SAM models are executed, computed values will be stored in the state file and will be available for subsequent model executions. Thus, the sequence in which models are executed has a direct bearing to the information available for a given models' execution.

As the value of any variable is stored in the SAM state file, it is compared to the nominal minimum and maximum limits defined for that variable. If an attempt is made to store a value which does not

lie within the nominal range, SAM will produce a warning message but will continue to use the value supplied in subsequent computations.

All values stored in the state file are in CGS units, and all internal computations are done also in CGS units. Unit conversion operations for input and output display are controlled externally to the state file, as governed by the type of quantity indicator stored in the file for each variable.

b. Default File

The default file contains a value for every input item in the state file, and at the start of each new run the initial contents of the state file are copied from the default file. Thus the default values, having the lowest source or priority code, are used only if no value is supplied by either the chemical properties file or the user terminal. A priority code 0, for no value present, exists only for correspondence with property file status codes, and cannot occur in the present configuration of SAM. The purposes of the default file are (a) to define the structure of the state file, and (b) to supply variable values so that a model can be executed regardless of whether every input item required by that model was specified by the user. This design also permits execution of SAM to continue even if errors are found by the user input processor, and the affected user data values cannot be stored in the state file. An indication in the output that a default value was used should be interpreted as a warning to the user that he has not specified a particular value required by a given model. He may then elect to specify that value and rerun SAM, or he may accept the results of the model based on the default value that

has been used if he judges that value acceptable.

c. Chemical Properties File

The chemical properties file contains the physical and chemical properties, currently for 900 hazard chemical substances. The properties of a given chemical are automatically accessed by the Property Data Processor, initiated by a user request specifying the recognition code of the discharged chemical.

The physical property file is arranged in sequential binary records. The first record on the file is a header record which identifies the version number, creation date and file label. The remaining records are those of chemical properties, appearing in ascending alphabetical sequence by chemical recognition code. Output is provided with each HACS run to identify the version of the property file that was accessed.

Each binary chemical properties record is arranged in two arrays. The first is a status code array and the second is an array of data values for each of the 74 items recorded for each chemical. Each of these properties has a status code indicating whether the data value associated with it is an exact value (status code = 3), an estimated value (status code = 2), or a missing value (status code = 0). Data values are transferred from the property file to the HACS state file only if the status codes are exact or estimated; missing property values are not transferred.

The data array contains the values for each of the properties in either numerical or alphanumerical data. All numeric data is stored on the property file in SI units and conversion to CGS units is performed automatically on transfer. A list of the 900 chemicals currently contained

on the file, along with their chemical recognition codes, is given in Appendix A.

d. Save File

The save option is an automatically controlled feature, initiated by the appearance of user selected options for RUN, RERUN and CONTINUE which are described in Section III.3

2. USER INPUT

SAM contains an interim interactive user interface module (UIM) to facilitate the use of the spill model from remote low speed computer terminals. During normal operations HACS displays prompt messages at the terminal, requesting input from the user that controls the overall sequence of operation. These start with the selection of the type of run, identification of the discharged chemical, and specification of the hazard assessment model(s) that are to be run.

As presently implemented, the UIM is functionally located between each assessment model and the HACS internal state file. That is, first user operations control the initialization of the state file, first with default data and then with optional physical property data. At the start of the execution of any particular model, the required user data is not necessarily contained within the state file. When the model attempts to retrieve a data item from the state file for computational use, the UIM first displays that value to the user and initiates a terminal input sequence for the data item. Users may either accept current values in the state file or enter new values. Once input, the data item is both stored in the state file and returned to the initiating model.

The UIM provides for free-format terminal input, and data entered by the user are validated as received. Diagnostic conditions are displayed, and users may correct errors before proceeding.

Overall, the data input requirements for the assessment models are quite complex. Data items for different models may either be similar or different. Within a single model, different data elements may be required depending on spill conditions or user options. By interfacing directly with each model, the UIM is able to request from the user only those data items that are actually required for the specific computation requested by the user.

3. BASIC PROCESSING STEPS

A basic execution involves interfacing with a number of files to collect the input required for SAM estimation models and to present the results of estimation model calculations to the user. Subsection 3.b of Section III introduces extended capabilities provided by SAM using options for RERUN and CONTINUE control; the discussion below is limited to basic RUN control only.

a. RUN Option

(1) Access Default File

SAM begins a basic run sequence by copying the contents of the default file from permanent disk storage to the internal memory space reserved for the state file. This defines a file dictionary for the contents of the state file and enters a value having a source or priority code of 1 for every variable which has been defined in the state file.

(2) Process User Input Control Data

The User Input Processor next conducts a dialog with the user terminal to obtain data which specify run control options, the recognition code of the discharged chemical substance, hazard assessment estimation route codes, and selection of system controlled options.

(3) Copy State File

Following completion of initialization for a single assessment run, the contents of the state file are copied to the internal memory space reserved for the save file. This file may be used to re-start subsequent assessment runs.

(4) Exercise Option to Access Property File

Users may enter all necessary physical property data directly, or may elect to have SAM obtain the necessary information by searching the physical property file which presently contains data for 900 hazardous chemical substances. Direct user input is necessary for chemicals not defined on the file and may be advisable if a larger series of runs are to be made using the same chemical. In any case, user values may always be supplied to override any item contained on the property file.

(5) Search Property File

The Property Data Processor takes the user specified chemical recognition code and controls a sequential search for a matching code on the property file. When found, all data defined (source codes 2 or 3) is read, decoded, and converted from SI units to CGS units for transfer to the HACS state file. The Property Data Processor also

performs the computation of all properties given as functions of temperature, at both ambient and boiling temperatures.

(6) Property Data Report

The operations performed by the Property Data Processor are summarized by printed output; a user option is available to suppress most of this output if desired. Since all defined property values are transferred, the report will reflect the property file content and whether these values are necessary for the user-specified estimation route. The audit reports produced by each assessment model will identify the specific property data used for input to the model. Diagnostic messages are not suppressed.

(7) Transfer Property Data to State File

The Property Data Processor transfers all chemical property values defined (exact or estimated) on the property file, and all functions of temperature which could be computed to the HACS state file. For each item, the status code of the value currently stored for a field is checked before the property value is stored. If present, user data or HACS-computed values will override values obtained from the property file.

(8) Initiate Model Executions

Using the model codes specified by the user for the estimation route data, HACS initiates a sequence of model executions. The system routines first locate the appropriate program code on a permanent disk file, load this into memory and then transfer control for execution.

(9) Assessment Model Data Input

As each assessment model is executed, the model retrieves each required data item from the state file. The current value may be either a default value or a chemical property value. If more than one assessment model is being executed or under RERUN or CONTINUE control, current values may also be previously computed or user input values. At the time of retrieval from the state file, the UIM conducts a dialog with the user terminal; users may either elect to accept the current value or enter a new value as may be appropriate.

(10) Assessment Model Execution

On completion of the model input operation, the actual hazard assessment computations are performed and the computed results are displayed. Addditional outputs in the form of tables or graphs may also be generated depending on user specified options. The output of each model is labeled using messages to denote the sequence of operations.

(11) Complete Execution of Prescribed Estimation Route

The HACS executive system continues to cycle through steps 8 to 10, executing each of the assessment models specified by the user until all calculations along the hazard estimation path have been performed. Each model obtains in sequence the necessary input data from the HACS state file and stores in the state file its computed results. In general, in the absence of overriding user data, some or all of the output stored in the state file by a rate model will be accessed as input for a model following in the estimation route sequence.

(12) Continue User Operations

After all models along the specified estimation route have been executed, the executive system resumes control to begin processing the next user specification for a chemical and hazard assessment path. The state file is initialized depending on the user selection of RUN, RERUN, or CONTINUE options and the above sequence of operations recycles starting with step 2. Computations continue until the user requests termination of the session.

b. CONTINUE and RERUN Options

Two additional types of basic hazard assessment runs may be performed to provide for interactive analysis, assessments using products of reactive chemicals, and selective control of overriding user data.

The basic RUN option, described above, follows a sequence in which initial default data values are replaced by physical property data; then a series of assessment models are executed to obtain and store computed results in the state file. During these operations, the sequence of model executions is fixed by the codes entered by the user; user data values in the state file will always override any values computed by rate models.

To illustrate the CONTINUE option, one or more assessment models might be executed using the RUN option to produce an assessment report plus an updated state file containing computed values, as well as the original set of user input data values. The CONTINUE option permits users to immediately follow this run with one or more additional runs starting with the full set of computed values previously obtained but

including new or revised user values. This permits selective override control for computed values, allows different portions of an overall hazard assessment situation to be run with different options for file control, output selections, path codes and even chemicals, and allows different user values to be substituted for the same variables at different locations along the assessment path.

The RERUN option originally provided for repeating a basic assessment RUN while at the same time modifying some of the original input data. In operations with the UIM, however, the use of the CONTINUE operation together with interactive user input directly to each assessment model now provides an equivalent function.

The RUN, RERUN, and CONTINUE options may be repeated indefinitely, within the computer time and line limits set for the HACS job. Users are cautioned, however, to note the sequences that are used to initialize the state file at the start of each type of run so that there is no confusion as to the nature (source) of the data that is used. These options will function even if given in sequences other than intended, and default values will be substituted automatically if necessary. Also, users are cautioned that during the transfer of physical property data items, if a state file already contains either computed or user values for property items, these will not be replaced or re-initialized by values read from the property file.

The HACS executive system controls the state file initialization sequences for all RUN, RERUN and CONTINUE options, and provides on the terminal output a message indicating the file status as EMPTY,

DEFAULT, USER, or COMPUTED, referring to the highest source code for any data item in the file.

SECTION IV

DISCHARGE CONDITIONS

The spill model specifically addressed in this manual computes the concentration of a water miscible liquid or solid at any specified point and given time for a continuous or instantaneous discharge into a lake, river, or estuary. All the chemical is assumed to go into solution with water. This same model can also be used for the dispersion of insoluble solids which are neutrally buoyant or whose settling times are large compared to mixing times. It can be used approximately for concentration predictions for those fluids which react with water or whose boiling point is less than that of ambient temperature.

In Section V, the specific instructions necessary to operate the model are given with illustrative system prompts, descriptions, and tables of data items with explanations. This section provides a general description of the types of water bodies, coordinate systems, types of release, and behavior on release.

1. TYPES OF WATER BODIES

When a water miscible liquid is spilled on a water surface, mixing takes place, thereby diluting the liquid. The mixing is caused by molecular diffusion in calm water and mass convection (turbulent diffusion) in streams, rivers, estuaries, and the sea. Mixing may take place preferentially in one direction, depending on the flow conditions, flow geometry, water density gradients, and the like. Because of the predominance of certain types of mixing phenomena in different regions of the navigational waters, the spill environments are broadly classified as lakes, non-tidal rivers,

tidal rivers, estuaries or salinity intrusion regions of tidal rivers, and open sea.

In non-tidal rivers the main agency for mixing is stream turbulence. In tidal rivers, estuaries, and also in the open sea, wave action becomes quite important in addition to the stream or current velocity. In estuaries and other regions where a density stratification of water due to salinity is likely to be found, mixing caused by the density-driven circulation becomes extremely important. However, since the velocities involved in these circulations are small and the area influenced by these kinds of flows is generally large, only long-time effects are important. For assessing the hazards caused by a relatively infrequent spill (even though the tonnage of the spill itself may be large) in such areas, the effects of salinity-driven mixing have been ignored.

In general, the receiving water bodies are treated as three-dimensional non-isotropic volumes, that is, turbulent dispersion is assumed to occur at different rates along the principal coordinate axes selected for the water body. Applicable methods for computing values of these dispersion coefficients are incorporated in the model, and, where necessary, simplifying assumptions have also been incorporated in the computerized version of the model. However, the form of the theoretical expressions as implemented continues to reflect the non-isotropic nature of the dispersion processes, so that different values of the turbulent dispersion coefficients can readily be used in place of internally computed values should suitable alternate generalized methods of computation become available.

The predominant types of receiving water bodies then are distinguished for the purpose of modeling by the predominant nature of the motion of the

water body:

- Still Water -- in which different dispersion currents may occur in different directions, but the water body is characterized by the absence of bulk motion of the receiving fluid (thus the reference to still water). Also, as implemented, the geometry presently incorporated for the still water case assumes that the boundaries of the water body are located far from the location of the spill so that unconfined dispersion occurs in three directions. The model therefore is only strictly appropriate for spills occurring in large lakes, or regions of open sea, far from shore, and in the absence of significant wind or wave action induced currents.
- Non-Tidal Rivers -- in which the characteristics of the water body are non-isotropic, with turbulent dispersion occurring at different rates in different directions, and where bulk fluid motion of the receiving water body occurs in one direction (downstream) at a uniform rate. In many cases the influence of turbulent diffusion in the longitudinal direction is commonly considered to be negligible with respect to the bulk fluid motion. Also, in addition, the river cross section is assumed to be bounded by channel banks and bottom so that the lateral spread of the chemical in the water may be confined. The longitudinal (downstream) direction is assumed to be unbounded.
- Tidal Rivers -- in which the same configuration is assumed as for a non-tidal river with the addition of a sinusoidal tidal

velocity component superimposed on the non-tidal river velocity.

a. Water Body Coordinates and Geometry

(1) Still Water

The coordinate system used for spills into still water (lakes and open sea) is shown in Figure 1. The origin of the coordinate system is

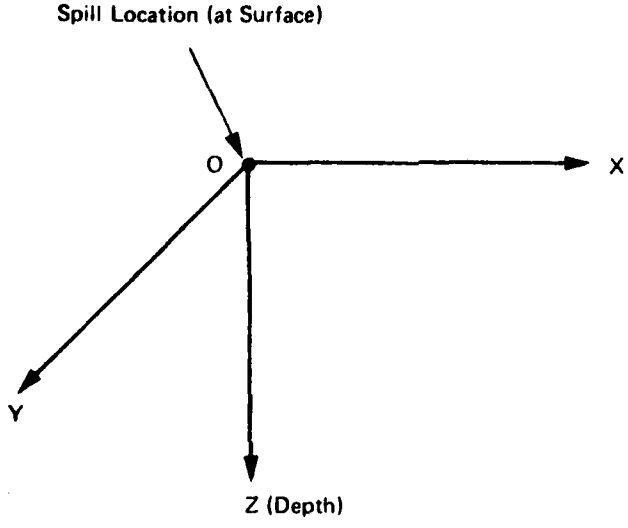


Figure 1. Still Water Coordinates

at a point on the surface of the water body, and x and y axes lie in the plane of the water surface and the positive z-axis is downward so as to form a right-handed orthogonal coordinate system. Since the dispersion is unconfined, the region of potential interest is given by all values of x and y, and values of $z \geq 0$ (for depth).

The origin of the coordinate system is taken at the location of the spill so that the coordinates of a point in the still water system also

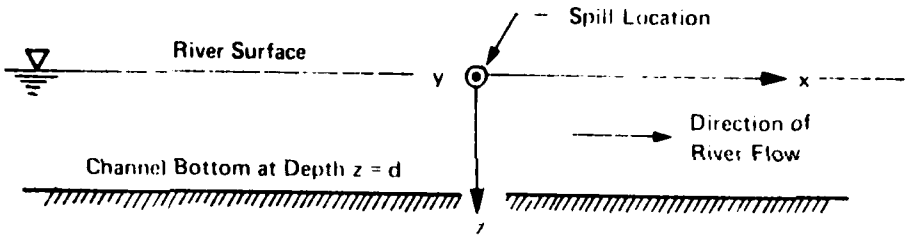
specify position relative to the spill. This is not the case for river system coordinates.

(2) River System Coordinates

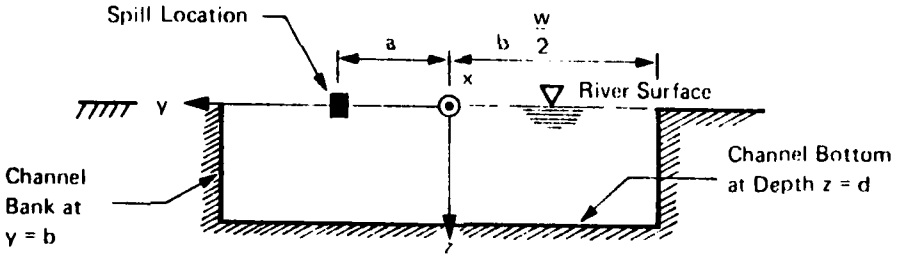
Figure 2 identifies the coordinate system (x,y,z) used for spills into both non-tidal and tidal rivers and illustrates the assumed river channel geometry. The river channel is assumed to be rectangular in cross-section, having a constant width w and a constant depth d. The origin of the river coordinate system is taken at the centerline of the river on the surface. The half-width of the river, the distance from the centerline to either bank, is denoted as b. In river system coordinates, the positive x axis gives downstream distance, positive z gives depth below the surface, and y is cross-stream so as to form a right-handed coordinate system.

For non-tidal rivers, the bulk fluid motion is assumed to occur in the x-direction, at a constant uniform cross-sectional velocity given as u. For tidal rivers, an additional sinusoidal tidal velocity is superimposed on the non-tidal velocity.

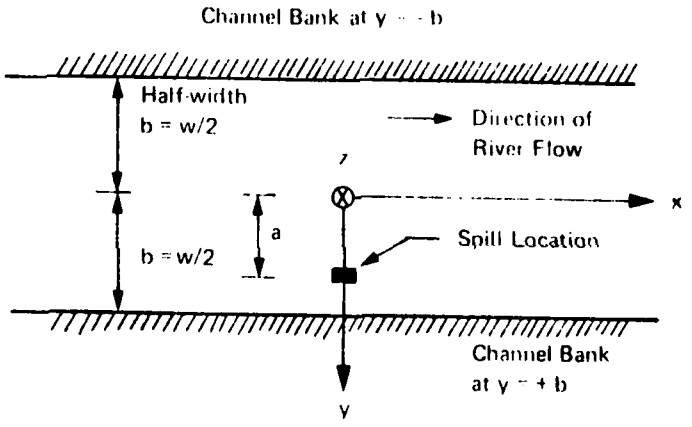
The location of a spill in a river is taken to be at the surface ($x = 0$, $z = 0$) at a point in the channel offset from the centerline by a distance given as a. Positive values of the offset a correspond to spill locations in the positive y direction. Since the coordinates of any position in the river, given in river coordinates, do not also specify position relative to the spill location (unless $a = 0$), a transformation is utilized for the general case of spills occurring at offsets from the centerline.



(a) Longitudinal Section of River



(b) Lateral Section of River



(c) Plan View

Figure 2. River System Coordinates

b. Observation Point Coordinates

In this context the observation point refers to the location (time and distance) in the coordinate system of the receiving water body at which the concentrations resulting from a spill of a chemical are to be obtained. The time at which the concentration at the observation point is desired is specified by the elapsed time from the start of the spill.

c. Coordinate Constraints

For spills in still water, the coordinates (x,y) of an observation point may be positive or negative, while the z coordinate (depth) must be greater than zero. Values of elapsed time less than zero should yield concentrations of zero at all locations. Although x, y, z, and t may take on large values, finite, but large, limits should exist beyond which computed concentrations should be zero; the values of these upper limits will, in general, depend on the behavior of the dispersing chemical.

Since the river system geometry is more complex, additional constraints are required. The location of the spill must be contained within the river channel:

$$-b \leq a \leq b$$

Symmetry could be used to restrict the allowed values of the offset, a, to only positive values of y; however, this is not necessary. The y coordinate of the observation point must also similarly be constrained to lie within the channel banks:

$$-b \leq y \leq b$$

The observation point must be located at or below the surface, but at or above the channel bottom:

$$0 \leq z \leq d$$

The coordinate of the observation point in the longitudinal direction, x, will have upper and lower limits depending on the behavior of the dispersing chemical and the type of model used. In some cases, at very short times after the start of a spill, some concentrations may occur for small negative values of x. As for spills in still water, both x and t may take on large positive values, but should also have finite upper limits beyond which only zero values of concentration can be obtained to within available numerical accuracy. For values of elapsed time less than zero, concentrations at all locations should also be zero.

The dimensions of the river channel, the half-width b (or the width w), and the depth d must be greater than zero. It is also necessary to constrain the bulk fluid flow such that the velocity u is non-zero.

(1) Confined or Unconfined Dispersion

For the lake or still water model, the spill is assumed to occur in a region of water far from shore so that the effects of the shore or bottom in confining the spread of a chemical in water may be neglected. In the case of spills in rivers, however, the channel banks or bottom may act to

restrict the dispersion of the chemical, and give rise to different regimes or subenvironments for inclusion in the models.

For the initial stages of a spill into a non-tidal river, at a point on the surface of the water sufficiently far removed from either bank, the spread of the chemical will occur in a nearly unconfined manner such that the effects of the channel banks may be neglected. During the initial stages of unconfined dispersion, the spill model utilizes a three-dimensional formulation of the dispersion equations to obtain values of the concentration at any point in the river cross-section; this form of the concentration equation is commonly referred to as a near-field model and applies for times close to the start of the spill when the effects of channel confinement are negligible.

Depending on the relative depth and width of the river and the location of the spill point with respect to the channel geometry, at some time after the start of a spill, the effects of the channel boundaries become more significant and the mixing will tend to become more or less uniform in either the horizontal direction, the vertical direction, or both. At some later time, complete mixing across the cross-section of the river can be assumed, and a simplified model, based on this assumption, can be used to obtain the cross-sectional average concentration. Such a model is referred to as a far-field approximation, or one-dimensional model, since the average concentration is assumed to be a function only of time and longitudinal distance from the spill point. The primary advantages of such a model are that the computations are significantly simplified for regions far removed from the spill point, and analytical approximations for very large times and distances are readily developed.

For the intermediate region of interest, between the near-field and far-field extremes, a two-dimensional model could be postulated based on uniform or nearly uniform cross-sectional mixing in one cross-sectional direction but not the other, with appropriate boundary conditions specified to govern the limits of applicability of the model. However, the effects of the channel banks and bottom may also be directly incorporated in the three-dimensional or near-field model by a method of superimposing contributions from virtual spill sources to satisfy the boundary conditions at the channel limits. This is the method that has been utilized for the spill model and, although there are some limitations since only the virtual sources having first order effects were included, a separate two-dimensional spill model is not required. In fact, if a sufficiently large number of virtual sources were included, the near-field model could also be used for large times or distances in place of the far-field model.

2. TYPES OF CHEMICAL RELEASE

The dispersion of a chemical in water follows from the behavior of solutions to the governing diffusion or continuity equation, subject to the initial conditions at the start of the release and whether the discharge takes place over an extended duration. Releases are characterized as point sources or distributed sources to indicate the initial spatial distribution of the released chemical. Relatively simple mathematical expressions are readily obtained for point sources in which a finite amount of chemical substance is initially introduced into an infinitesimally small volume of the receiving water body; these models have a disadvantage in that the estimated concentration at the spill location has an infinite value initially and will exceed the density of the spilled chemical for some time after the

start of the spill. Distributed sources, on the other hand, refer to releases which take place over a finite dimension, which may be a line (1-D), area (2-D), volume (3-D), or any combination of these. Distributed sources have a disadvantage of requiring a description of the geometry of the distribution, and any arbitrary assumptions would increase the complexity and uncertainty of model use in different situations. As the distance from the spill location increases, localized effects at the spill origin become diminished and the concentrations approach those of a point source. Accordingly, the spill model assumes the discharge occurs as a point source, but includes a constraint restricting computed concentrations to values not exceeding the density of the chemical.

The second fundamental characteristic of the spill process is whether the spill of the entire amount of substance occurs instantaneously or continuously over some finite duration. Commonly, continuous spills are assumed to take place over long durations, and the initial rise time as the dispersing chemical spreads through the receiving water body is usually neglected. Thus, most solutions obtained for continuous spill conditions represent steady state concentration distributions where, subject to the conditions of the start and cessation of a release of finite duration, the steady state concentration at any observation point x, y, z is independent of time.

a. Instantaneous Point Source

The instantaneous point source is the conventional approximation to the type of release associated with a very short venting of material, such as might be associated with an explosion, tank car derailment, or similar

occurrences of short duration. The term "instantaneous point" is a mathematical simplification since even a small, rapid explosion will have finite time and space dimensions. The slug, or mass of spilled chemical, once formed, moves away from the source with a speed and direction determined by the prevailing bulk fluid velocity of the receiving water body (as in the case of a river). In still water, the mass of the spilled chemical remains centered about the spill location; only turbulent dispersion or molecular diffusion takes place and this simplified behavior is not described further.

The mean speed and direction of the slug can be expected to change from the original values during its travel as the pattern of river currents in which it is embedded changes with time. Since specification of river current variations is not practical within the objectives of a generalized spill model, a limiting assumption is employed that for non-tidal rivers the river flows with a constant cross-sectional velocity so that the center of mass of the spilled slug moves downstream, along a longitudinal line from the spill location, at a constant rate equal to the river velocity.

As the slug moves, it will expand about its center owing to the action of turbulent fluctuations. If an idealized slug is embedded in a uniform turbulent field in which all the turbulent elements are smaller than the dimensions of the slug, the entire mass of spilled chemical will be carried downstream in a uniform manner. The slug will grow in size as its edges are mixed with the water by turbulence. This growth is accompanied by a proportional decrease in concentrations within the slug.

If the slug is originally embedded in a field of turbulent elements that are considerably larger, the movement of the slug will occur mainly

by bulk transport driven by the turbulent elements, with relatively little dispersion or decrease in concentration within the slug. If the slug is instead embedded in eddies of approximately the same size, diffusion will be quite rapid and the concentration within the slug will decrease rapidly.

The downstream distribution of the spilled substance after it has been dispersed is frequently expressed in terms of exposure, or the time integral of the concentration as the slug passes the observation point.

b. Continuous Point Source

Continuous point sources give good approximations to tank venting from small holes, fissures, or pipes. The approximation of the true source configuration becomes increasingly better as the distance at which the concentration is observed grows increasingly large compared with the dimensions of the source.

A continuous release may be considered to be made up of an infinite number of slugs released sequentially with a vanishingly small time interval between slugs. Initially each slug moves with the river current at the moment of release. The quantity of material released is usually expressed in terms of a release rate, and the downstream material distribution is usually expressed in terms of average concentration over the period of release. Linear dimensions of the dispersing material perpendicular to the longitudinal axis, running downstream from the spill site, are often given in terms of the standard deviation of the concentration distribution since the average cross-sectional distribution, in the absence of significant boundary effects, is usually close to a normal curve with boundaries at infinity.

Since the plume from a continuously maintained point source expands both laterally and vertically with downstream distance from the source, the centerline concentration along the downstream axis from the spill point will decrease continuously with distance. The rate at which this decrease occurs will depend on the magnitude of the turbulence.

For the purpose of the water dispersion model, an adequate concept of a continuous release is that of a series of an infinite number of instantaneous releases, creating a plume in the downstream direction of a dispersing chemical mass. Concentrations are reduced with distance from the spill in both the longitudinal and cross-stream directions, however, for long duration events, the concentration obtained at any observation point is a steady state value and not a function of time.

3. CHEMICAL DEGRADATION ON RELEASE

The form of the continuity or governing diffusion equation provides for limited modeling of non-conservative effects or decay or degradation with time of a released chemical in the environment. The rate of loss is assumed to be proportional to the concentration of the substance, and the factor of proportionality is taken as a decay or rate constant, k, having dimensions of $(\text{time})^{-1}$.

Solutions of the diffusion equation for the Gaussian model give the result, for an instantaneous release, that the concentration distributions depend on the total mass of substance in the diffusing media, and that mass is reduced according to e^{-kt} where k is a decay factor or rate constant for overall degradation of chemical in environment, and t is the elapsed time from release.

This results in a description of the time-dependent degradation process that is simply related to the elapsed time from release and is a usual limitation of a Gaussian model. The influences of chemically interacting sources, or source components, of formation reactions involving several primary or secondary pollutants, or the photochemical effects are normally beyond the scope of these models.

The exponential e^{-kt} gives the ratio of the total amount of substance in the diffusing media at any time to the amount initially present. Values of the exponential function vary from 1 to 0 as t becomes very large.

If no decay or degradation is assumed to take place, then for k = 0, the value of the function is 1.0 for all values of time; the total amount of substance in the environment is constant and equal to the amount originally released at time t = 0.

For non-zero values of k, decay occurs rapidly over a short range of values of kt. The concentration distributions are proportional to the total mass in the environment, and this factor varies from 1.0 for kt = 0 to approximately 0.05 for kt = 3.0 (only 5 percent of the mass originally released remains at kt = 3). Thus, for large values of k, the time over which finite concentrations may exist will be limited by the time over which e^{-kt} has a non-negligible value.

Half the mass originally released remains at a time $t_{1/2}$ given by:

$$\frac{1}{2} = e^{-kt_{1/2}}$$

so that

$$t_{1/2} = \frac{\ln(2)}{k} = \frac{0.693}{k}$$

where $t_{1/2}$, the time for one-half of the original amount of substance to decay, is known as the half-life. If data is available expressed by half-life, the appropriate rate constant for use in the spill model is given by:

$$k = \frac{0.693}{t_{1/2}}$$

where the units of the decay constant are the reciprocal of the units in which the half-life is given.

Reduction of substance in the environment may be the result of more than one decay process. If separate degradation processes (such as oxidation, biodegradation, hydrolysis, photolysis, etc.) are estimated in terms of separate rate constants, the overall decay coefficient k is obtained as the sum of the individual rate constants. The half-life of the material is obtained as ln(2) divided by the sum of the rate constants. If the degradation processes are described by separate half-lives, then conversion to individual rate constants is required before the summation.

Half-life estimates for the degradation of hydrazine fuels in the aquatic environment appear to be on the order of 10 to 1000 hours. Taking a half-life of 100 hours gives a nominal value for the decay coefficient of 6.93×10^{-3} hours or 1.15×10^{-4} minutes. At this value, an elapsed time of approximately 430 hours would be required to reduce the total amount of a spilled substance to 5 percent of its initial mass.

However, experimental studies have also concluded that slow degradation rates occur in the absence of added catalysts and, as a result, that hydrazine should be assumed to be conservative in modeling aqueous spills. Furthermore, to the extent that decomposition in water does occur, many of the reaction products may also be harmful; since the model does not have the capability of including reaction products, further justification is suggested for the conservative approach to ignore the separate reaction products and use a decay coefficient of zero.

SECTION V

USER OPERATIONS

Once execution has been started, the spill model proceeds through a sequence of steps, displaying messages to the user terminal, and reading and validating user input data typed at the terminal. The types of operations performed during runs of the spill model generally consist of run set-up, input of specific model data, model execution, preparation and printing of output tables and/or plots, and modification of input data for model reruns.

Terminal interaction with the spill model is provided by means of an interim interactive user interface module. This module provides a capability of entering data in a free-format mode and provides a standard sequence of operations for input of each user data item. These operations are:

(1) Display of current data value.

(2) Request user option to change current value.

(3) Accept and validate optional user input.

(4) Repeat steps 1 and 2.

This gives a user the capability of re-entering a data value if the previous entry was incorrect.

Overall control is provided by an executive module which proceeds step-by-step through the selection of various options and processing of user input data. A majority of the user input operations consist of entering either integer values or real values with associated unit labels (dimensions). The paragraphs that follow first describe these basic procedures; then a separate section on execution control describes the overall framework within

which these procedures are utilized.

1. INPUT PROCEDURE FOR INTEGER VALUES

Certain data items used in the spill model have integer values and are used to select one out of several different options. Generally, a request for user input of an integer data item is preceded by a display listing the different options that are available. Following this display, the integer value input procedure starts with the message:

(1.1) (field number) (name) = (value) (unit) IS A (type) VALUE

where (1.1) is a message reference number, not appearing in the actual display but used in this text for illustration. Each data item in the system is identified by both a four digit field number and a name of up to 12 characters. The appropriate field number and name are automatically inserted in the above message by the model.

The current value for the integer variable is also displayed. All integers are non-dimensional so the unit display in the message is always given as "ND."

The space in the message for type is filled with a code word which indicates the origin of the value currently stored internally. Possible types of values are:

Default - the value is selected from an internal table of initial values in the absence of any other input.

Estimate - current value was obtained from the external file of chemical property data and is an estimated value.

Chm prop - the current value was obtained from the external file of chemical property data and is an exact (referenced) value as opposed to an estimated value.

Computed - the value currently stored was obtained from the previous execution of a model which set the variable to the value shown.

User - the current value was stored from input entered by the user.

System - the value was set internally by the executive portion of the system to override all other input sources.

Generally, the use of integers is somewhat limited, and commonly only default, computed, and user values will appear. Users should refer to Section III for additional information on the internal priority scheme for data storage and selective overrides. Following the display of the current value of an integer variable in the message (1.1), the system then requests whether the user would like to specify a different value to be used in place of the current value.

(1.2) DO YOU WANT TO CHANGE THIS VALUE?

(1.3) ENTER YES OR NO (Y/N):

Acceptable user responses are to type Y or N followed by a carriage return. Actual input may be typed anywhere on the line at the terminal, and any words are acceptable as long as the first letter is Y or N.

If the input line from the terminal is blank, or a word is typed that does not begin with the letter Y or N, the system gives the message:

(1.4) WHAT?

and message (1.3) is then repeated.

If the user types N or NO, followed by a carriage return, the system retains the value displayed in message (1.1) and the input procedure for this variable is completed.

If the user types Y or YES in response to message (1.3), the input procedure for the variable continues.

(1.5) VALUE RANGE IS min TO max

where the range limits (min,max) are automatically inserted in the message display by the system. Each variable or data item has a set of nominal range limits associated with it, and these are used to generate warning messages to to the user for possibly invalid values. Since almost all integer values are used to select one from a set of predetermined options, attempts to enter integer values outside the nominal range will cause serious execution

errors.

(1.6) ENTER INTEGER VALUE:

Valid integers which can be read by the system consist of an optional sign (+ or -) followed by one or more decimal digits. The integer is terminated by the first blank character encountered. Valid examples include -99, +5, 52, 0, etc. As many blanks as desired, or none, may precede or follow the value typed.

The interim interactive user interface module does not presently contain a capability of detecting or preventing numeric overflow. That is, the largest value that can be stored depends on the word structure of the computer system being used, and errors may result if entry of very large numbers is attempted.

If the user simply keys a carriage return, the system assumes that the user may not wish to proceed with the input, and processing returns to repeat message (1.2). This gives the user an opportunity to abort an input procedure and retain the current value of a variable.

If the input keyed by the user at the terminal cannot be decoded as a valid integer, for example, if an alphabetic letter is typed instead of a digit, the system responds with:

(1.7) WHAT? (INTEGER SYNTAX ERROR)

Message (1.6) is then repeated to request correct input

from the user. Note that, on most terminals, the backspace key can be used to correct errors before a value is entered (by hitting the carriage return).

If the data item entered by the user in response to message (1.6) is successfully read as a valid integer, the value read is then compared to the nominal range limits. If a limit is exceeded, the system will respond with:

(1.8) WARNING, INPUT VALUE = (value) NOT
WITHIN NOMINAL RANGE OF (min) TO (max)

This message indicates a warning condition only and the value of the variable displayed will be used unless subsequently changed by the user.

At this point the user input value for the requested integer variable has been read and stored by the system, and the value actually stored is displayed to the user for verification by a repeat of message (1.1). This is then followed by messages (1.2) and (1.3). A yes response to (1.3) will allow the user to re-enter the value, and a no response completes the input procedure for the data item.

2. INPUT PROCEDURE FOR DECIMAL VALUES

The input procedure for decimal values is quite similar to that for integer values, the main differences being in the format of the decimal values and in optional units of measure which are available. Almost all decimal values used in the spill model are dimensioned quantities, with conversions applied between external and internal representations. The

input sequence starts with a message:

(2.1) (field number) (name) = (value) (unit) IS A (type) VALUE

where the individual items for the variable are as described for integer values in Subsection V.1, and are automatically inserted in the message by the model. Decimal values do have dimensions or units of measure, and these are defined by the label inserted in place of (unit) in the message. An appendix to this manual defines the full set of unit labels which are currently incorporated in the system.

Each data item may have from one to four different unit labels assigned, each label defined within a system of units (CGS, SI, ENG for English, and MXD for mixed). An integer data item (field number = 3019, field name = UNIT SELECT) is used to control the dimension of the value displayed by selecting one system of units or all systems of units. If one system of units is selected, then all messages (2.1) will display data item values in appropriate units selected from the specified system of measure. If all systems of units are selected by the user, the message (2.1) is followed by additional messages in the form:

(2.2) = (value) (unit)

where the value of the data item is displayed in each defined different unit (up to a maximum of four different values).

The system then requests a user option to change the current value by displaying:

(2.3) DO YOU WANT TO CHANGE THIS INPUT VALUE?

(2.4) ENTER YES OR NO (Y/N):

If the user response is blank or invalid, the system responds with:

(2.5) WHAT?

and message (2.4) is repeated.

If the user types N or NO in response to (2.4), followed by a carriage return, the system retains the value displayed in messages (2.1) and (2.2) and the input procedure for this variable is completed.

If the user types Y or YES in response to (2.4), the input procedure continues with:

(2.6) UNITS ARE /$unit_1$/$unit_2$/$unit_3$/$unit_4$/

where up to four different unit labels available for the particular field are displayed. The first label in the display is particularly significant since it is designated as the default unit that is used in the absence of user specification.

(2.7) ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:

Valid decimal values which can be read by the system consist of an optional sign (+ or -) followed optionally by one or more decimal digits, a decimal point, additional digits and an optional exponent. If present, the exponent is defined as the letter E, followed immediately by

a valid integer. Blanks are used as separators, so the decimal number may not contain embedded blanks. Valid examples include 29.5, -31.678 etc. As many blanks as desired or none may precede or follow the value typed.

The interim interactive user interface module does not presently contain a capability of detecting or preventing numeric overflow. That is, the largest value that can be stored depends on the word structure of the computer system being used, and errors may result if entry of very large numbers is attempted.

If the user is entering a value in the default unit, then it is only necessary to type the decimal value followed by a carriage return. If the value is entered in one of the other units, then the value is followed by at least one space and the appropriate unit label is typed (and followed by a carriage return). Since the system performs units conversions by comparing the user input label to the entries in the unit list in message (2.6), the user entry for the unit label, if present, must exactly match one of the labels in (2.6).

If the user simply keys a carriage return in response to (2.7), the system assumes that the user may not wish to proceed with the input, and processing returns to repeat message (2.3). This gives the user an opportunity to abort an input procedure and retain the current value of a variable.

If the input keyed by the user at the terminal cannot be decoded as a valid decimal value, the system responds with:

(2.8) WHAT? (DECIMAL SYNTAX ERROR)

If the error occurs in the exponent of a decimal value, message (1.7) also is given. Following an error condition, message (2.7) is repeated to request correct input.

If the decimal value entered by the user passes the syntax check, the system then checks the unit label. If the user has not entered a label, the default unit from the first entry of (2.6) is assigned. If the user has entered a label, it is compared to the list of (2.6). If the unit label is incorrect, the system responds with:

(2.9) UNIT LABEL (input) IS INVALID

and processing returns to message (2.6).

If the unit label is correct, the user input decimal value is converted to internal (default) units and displayed:

(2.10) INPUT CONVERTED TO UNITS OF (unit) IS (value)

After conversion, the stored decimal value is compared to a set of nominal range limits and if a limit is exceeded the system displays a diagnostic message:

(2.11) WARNING, INPUT NOT WITHIN NOMINAL RANGE OF (min) TO (max) IN (unit)

This message indicates a warning condition only and the value of the variable displayed will be used unless subsequently changed by the user.

At this point the user input for the requested decimal value has been read and stored by the system, and the value stored is displayed for user verification by a repeat of message (2.1). This is then followed by messages (2.2), (2.3), and (2.4). A yes response to (2.4) will allow the user to re-enter the value, and a no response completes the input procedure for the data item.

SECTION VI

EXECUTION CONTROL

1. STARTING THE PROGRAM

Execution of the spill model starts with the system display of the message:

(3.1) HAZARD ASSESSMENT COMPUTER SYSTEM
EXECUTION STARTED ON date AT time

where the values of the current date and time are written with the message. Next the system initiates two sequences of operations: (a) user selection of run options and model specification, and (b) user input of specific model data using the standard input procedures previously described.

(3.2) ENTER RUN REQUEST, OPTIONS ARE RUN/RERUN/CONTINUE/END

The system requests that the user enter a code word to describe the type of run to be performed. A correct response is for the user to type one of the words RUN RERUN CONTINUE or END followed by a carriage return. Spaces may precede or follow the control word typed.

If the input line typed at the terminal is blank (only a carriage return was typed), the message is repeated. If the response to message (3.2) cannot be correctly interpreted by the system as a valid code word, then the following message is displayed:

(3.3) WHAT? (RUN REQUEST ERROR)

and message (3.2) is repeated.

If the user response for the run request is END, further execution of the model is terminated, and the system responds with the message:

(3.4) END OF HACS RUN

Further control for the terminal operation then returns to the computer operating system, and the user might normally log-off the system.

If the user response for the run request is one of RUN RERUN or CONTINUE, internal parameters are automatically set to control the initialization of state file values, and an informative message is displayed. Processing proceeds to the selection of the model and chemical.

(3.5) ENTER ASSESSMENT MODEL LETTER CODES (A-Z/II/RR/SS):

For the current installation of the spill model, users should only type the letter P followed by a carriage return. Entry of any other letter, if also included in the above list, will cause an execution error since the assessment models other than P have been removed from the installation.

A second version of the system is available, however, for limited access in which the full set of model letter codes can be utilized. Users should refer to the U.S. Coast Guard User Reference Manual for appropriate methods of

selecting multiple assessment letter codes.

Entry of any letter or combination of letters not included in the above list will cause a diagnostic message to be displayed by the system. User input is again requested by a repeated display of (3.5); a similar action occurs if the user input is blank.

Once a correct response has been entered by the user, the system re-displays the model letter code at the terminal for verification.

(3.6) ENTER CHEMICAL RECOGNITION CODE:

The expected user response is to type the three-letter chemical recognition code for the chemical of interest. Appropriate codes for the hydrazine family fuels are:

DMH = unsymmetrical dimethyl hydrazine

HDZ = hydrazine

MHZ = methylhydrazine

The complete set of 900 codes which can be used with the current version of the system are listed with the chemical names in Appendix A.

If a code is not entered (user input from terminal is blank), message (3.6) is repeated. Otherwise, the system saves the three-letter code typed by the user. The code entered is not immediately validated since user options regarding access of the external physical property data base must first be obtained.

(3.7) OUTPUT OPTIONS ARE:

0 SELECT ALL UNITS

1 SELECT CGS UNITS

2 SELECT SI UNITS

3 SELECT ENGLISH UNITS

4 SELECT MIXED UNITS

Input procedure for data item 3019, UNIT SELECT.

The system displays message (3.7) then performs the standard input procedure to obtain a value in the range 0 to 4 from the user for the data item UNIT SELECT. This item is used to control the units or dimensions in which other data items will be displayed during the remainder of the run. A value of 1, 2, 3, or 4 will cause only a single display to be produced, with the value given in the display in units appropriate for the specified system. A value of 0 will cause each display of data items (real values) to consist of four lines, one for the value in each system of units. Since all integer data items are treated as non-dimensional quantities, these items are always displayed in a single line independently of the value selected for this option.

(3.8) OUTPUT OPTIONS ARE 0 = SUPPRESS, 1 = SELECT

Input procedure for data item 3002, PLOT OFFLINE:

This option is not available in the installed version of the model which operates through the interim user

interface module to an interactive user terminal. Instead, plotted displays are produced directly at the terminal. The value of zero pre-stored in the system should not be changed by a user.

(3.9) OUTPUT OPTIONS ARE 0 = SUPPRESS, 1 = SELECT

Input procedure for data item 3011, READ PROP:

This option is available to suppress or to select access and retrieval of data from the external file of chemical property data for the chemical entered in response to message (3.6). Most models other than P will normally require access to this file. However, for spills into non-tidal rivers and estuaries, access to this file may be omitted if the user provides the density of the chemical as a direct model input (refer to following section). If the external file is not accessed, no further validation of the chemical recognition code occurs, and any code may be entered with (3.6). If the file is accessed, then the code entered with (3.6) must be defined on the file.

(3.9) OUTPUT OPTIONS ARE 0 = SUPPRESS, 1 = SELECT

Input procedure for data item 3018, PROP REPORT:

If the option to access the external property file is selected, then an additional option is provided to control the type of terminal display which is generated during the retrieval operation. For interactive terminal operation with model P, using terminals that are limited to

an 80-character line length, this option should not be selected. The full report is lengthy, requires in excess of 80 characters per line for display, and is not essential since the information actually required by the model is displayed during the model execution.

Following completion of user input for (3.9), then if the option to retrieve chemical data has been selected, the system starts the search of the file for the requested chemical. This status is indicated by:

(3.10) STARTING SEARCH OF HACS FILE FOR PHYSICAL PROPERTIES OF CHEMICAL code

where code is inserted as the three-character recognition code specified by the user.

(3.11) FILE OPENED HAS ID =

where the file identification, version number, creation date, and back-up identification are displayed for the file actually being accessed. This message defines for the user the identification of the file actually being accessed and provides for user interpretation of results if more than one version of the file has been created with differences in content.

The search of the physical properties file, if selected, has three possible outcomes: (a) the file is searched completely and the requested chemical is not found, (b) the position on the file where the requested chemical

should exist has been passed, or (c) the requested chemical is found. If either condition (a) or (b) occurs, the user-specified chemical recognition code is in error, and one of the following messages is displayed:

(3.12) *****ERROR - UNABLE TO FIND CHEMICAL
SEARCH TERMINATED BY END OF FILE

or

(3.13) *****ERROR - UNABLE TO FIND CHEMICAL
SEARCH TERMINATED AFTER PASSING EXPECTED ALPHABETICAL POSITION

following either of these conditions, the system displays:

(3.14) CHEMICAL code WAS NOT FOUND ON FILE

and processing returns to (3.6) to obtain a correct code from the user. The user must enter a code in response to (3.6) but then may also elect to suppress the file access when (3.8) is repeated.

If the search of the property file is successful, an abbreviated report is automatically displayed:

(3.15) PHYSICAL PROPERTY DATA RETRIEVED FOR CHEMICAL code
NAME =
PATH CODES =
SHIPPING STATE =

where entries in the display are obtained from the file. If the detailed report of the property data transfer has not been selected, then processing proceeds next with the input procedure for model P.

If the detailed report was requested, then additional displays are generated by the system at this time; these include conversions of data items from SI to CGS units and the computation of temperature-dependent properties. Users are referred to specific documentation in the U.S. Coast Guard HACS Users' Reference Manual. In addition, if access to the property file is selected, the system requests input for the ambient water temperature, and if the detailed report is selected, the system also requests input of the boiling temperature of the selected chemical. Both of these items are used for the computation of temperature-dependent properties during the actual transfer of property data to the HACS state file.

Following completion of the run specification input, and retrieval operations with the external property file, the executive portion of the system controls the sequence of execution of the models specified by the user response to message (3.5). For the spill model, P, the initial message is:

(3.16) MODEL P IS NOW BEING EXECUTED.

THE INPUTS REQUIRED FOR THIS RATE MODEL ARE ...

The number and type of model input data items depends on the type of water body and the type of discharge condition. Messages (3.17) and (3.18) are given at the start of the model input procedure to obtain user specifications for these items.

(3.17) WATER BODY OPTIONS ARE:

1 STILL WATER

2 NON-TIDAL RIVER

3 TIDAL RIVER

Input procedure for data item 2028, WAT TYPE P/R

The value specified by the user during this input procedure selects both the appropriate portion of the spill model and the specific input data requirements for that portion.

(3.18) SPILL TYPE OPTIONS ARE:

0 INSTANTANEOUS

1 CONTINUOUS

Input procedure for data item 2029, SPILL TYPE P:

Instantaneous liquid spills are characterized by the total quantity of mass released instantaneously, and this value is entered by the user for data item 4002, TOT MASS LIQ. Continuous spills are characterized by both the total mass of liquid released, and, in addition, the rate at which the mass is released (data item 4049, LIQ FLWRATE).

Next, the model initiates a user input procedure for each of the required data input items. Table 1 and Section VI, Subsection 2, following, describe each of these items. The actual user input of these items is controlled in sequence by the model using the

TABLE 1. MODEL DATA ITEMS

Usage			FIELD NUMBER	FIELD NAME	ALLOWABLE UNITS
Still Water	Non-Tidal River	Estuary			
•			1002	MOLEC WEIGHT	G/GM KG/KGM LB/LBM
•			1003	BOIL TEM LIQ	C K F
•	•	•	1004	DENS LIQ AMB	G/CM3 KG/M3 LB/FT3
•			1021	LIQ DENS BP	G/CM3 KG/M3 LB/FT3
•			1025	CRIT TEMP	C K F
•			2023	WATER TEMP	C K F
•	•	•	2039	CONC PT X	CM M FT MI
•	•	•	2040	CONC PT Y	CM M FT MI
•	•	•	2041	CONC PT Z	CM M FT MI
•	•	•	2042	TIME CONC PT	S MIN HR
	•	•	2044	RIVER DEPTH	CM M FT MI
	•	•	2045	RIVER WIDTH	CM M FT MI
	•	•	2046	OFF DIST	CM M FT MI
	•	•	2047	STREAM VEL	CM/S M/S MPH KNOTS
		•	2048	TIDAL VEL	CM/S M/S MPH KNOTS

TABLE 1. MODEL DATA ITEMS (CONCLUDED)

Usage			FIELD NUMBER	FIELD NAME	ALLOWABLE UNITS
Still Water	Non-Tidal River	Estuary			
		•	2049	TIDAL PERIOD	S MIN HR
		•	2050	PHASE LAG	S MIN HR
•	•	•	2051	DECAY COEFF	/S /MIN /HR
	•	•	2052	MANNING FACT	ND
•	•	•	4002	TOT MASS LIQ	G KG LB TN
*	*	*	4049	LIQ FLWRATE	G/S KG/S LB/S TN/HR
•			2043	DIF COEF H2O	CM2/S M2/S FT2/S

(*)The liquid flow rate is required for all three water body types only if the spill has been specified as continuous.

procedure described in Section V, Subsection 2. After all data items from Table 1 have been entered, the system displays:

(3.19) OUTPUT OPTIONS ARE:

0 SUPPRESS

1 CONC VS TIME AT x, y, z

and for spills in non-tidal rivers only

2 MAXIMUM CONC VS DISTANCE

3 BOTH OF THE ABOVE

The message is followed by input procedures for data items 3008, PLOT FLAG P, and 3015, TABLE FLAG P, for the user to either select or suppress a combination of graphic and tabular outputs for the particular run conditions. If any of these output reports are selected, the system also requests input from the user for data item 2037, MAX TIME CONC; this item is used to scale the length of elapsed time over which the displayed concentrations are to be computed.

Prior to executing the model with the user specified data, the system first examines the status codes associated with each data item that will be used in the computations. If the user has not been able to provide a specific input value for each item, and the system has selected an estimated value from an internal default data file, the following message will be displayed:

(3.20) WARNING - MODEL P IS USING DEFAULT VALUES

Under this condition, the model will continue to execute however, the user should review the input data to determine which input items are being used with default data, whether the default values appear to be realistic for the particular scenario, and whether actual values for these items can be obtained or estimated. The significance of default data values or of any input item for which there is some uncertainty can be evaluated by making a series of model runs using different values of these items.

(3.21) THE RESULTS OF MODEL P ARE ...

The initial execution of the model always gives the estimated concentration at the user specified observation point (x,y,z) and elapsed time t for the particular spill conditions. Within the framework of the overall HACS series of models, the computations performed at this point obtain results that may be required as inputs to different models which may be run subsequently.

For chemicals which are diluted with water before they are spilled, it is necessary for the user to multiply the computed concentration by the fraction of the spilled solution which consisted of the chemical. For example, if 28 percent hydrochloric acid is spilled instead of 100 percent hydrochloric acid, the computed concentration as displayed should be multiplied by 0.28 to obtain the actual value.

(3.22) THE EXECUTION OF MODEL P IS COMPLETED.

Following this message, any optional tables or plots which may have been requested by the user in response to message (3.19) are produced and displayed.

After the production of the optional output, all other models in the current version of HACS then return control to the executive portion of the system which will either initiate execution of another model selected by the user or request a new run option from the user. An additional cycle has been implemented in the spill model (P), however, that permits users to obtain additional optional output for the spill conditions previously entered.

(3.23) DO YOU WISH TO RE-RUN WITH A

NEW OBSERVATION POINT?

(3.24) ENTER YES OR NO (Y/N):

If the user response is not Y (or YES) or N (or NO) or is blank, a message (WHAT?) is displayed and message (3.24) is repeated.

If the user response is Y or YES, the model repeats the input procedure for the data items, specifying the coordinates of the observation point:

2039, CONC PT X

2040, CONC PT Y

2041, CONC PT Z

2042, TIME CONC PT

and then re-enters the model processing sequence with message (3.19) to request the selection of output options from the user. Message (3.19) is then followed by (3.20) and so forth, obtaining the new set of optional outputs and arriving again at messages (3.23) and (3.24). There is no internal limit on the number of these model cycles that can be performed.

If the user response to message (3.24) is N or NO, the control of the spill model is terminated, and the executive portion of the system repeats message:

(3.2) ENTER RUN REQUEST, OPTIONS ARE RUN/RERUN/CONTINUE/END

and the user may either continue operating the model with different data, or may terminate the session by typing END.

2. MODEL DATA REQUIREMENTS

Table 1 gives a summary of the data items that are required for each water body type, and defines the field number, field name, and allowable units for each item. Appendix D contains additional information defining the unit abbreviations. Further discussion and explanation of each input item is given below.

1002, MOLEC WEIGHT

The molecular weight of the spilled chemical is required only for spills into still water and is used in the computation of the diffusion coefficient.

1003, BOIL TEM LIQ

The boiling point of the spilled chemical is required

only for spills into still water and is used in the computation of the diffusion coefficient.

1004, DENS LIQ AMB

The density of the spilled chemical at ambient temperature is used by the model for all three water body types. Concentrations near a spill location, because of the assumed point source behavior, may be computed to exceed the density of the chemical. The model then applies a constraint limiting the concentrations not to exceed the density. Depending on the option selected for retrieval of chemical property data, the initial value for this item may either be a default value, or computed from physical property data at a temperature given by item 2004, TEMP START.

1021, LIQ DENS BP

The liquid density of the spilled chemical at its boiling point is required only for spills into still water and is used in the computation of the diffusion coefficient.

1025, CRIT TEMP

The critical temperature of the spilled chemical is required only for spills into still water and is used in the computation of the diffusion coefficient.

2023, WATER TEMP

The temperature of the receiving water body, as obtained from this data item, is required only for spills into

still water, and is used in the computation of the diffusion coefficient. Note that the liquid density computation from physical property data utilizes item 2004, TEMP START.

2039, CONC PT X

The downstream distance from the spill location at which the concentration of the spilled chemical is to be computed (x coordinate of observation point).

2040, CONC PT Y

The cross-stream position, measured from the center of the river, at which the concentration of the spilled chemical is to be computed (y coordinate of observation point).

2041, CONC PT Z

The depth from the surface at which the concentration of the spilled chemical is to be computed (z coordinate of observation point). Positive values of z specify depth below the surface.

2042, TIME CONC PT

The elapsed time from the start of the spill at which the concentration at the observation point (x,y,z) is to be computed.

2044, RIVER DEPTH

The mean depth of the water in the river channel. The coordinate z should not exceed the river depth.

2045, RIVER WIDTH

The mean width of the water in the river channel. The coordinate y should not exceed one-half the river width in magnitude (the coordinate may be positive or negative).

2046, OFF DIST

The cross stream location on the surface of the water body at which the discharge occurs, measured from the center of the river channel in the same direction as the coordinate axis y, i.e., an offset distance and a y coordinate having the same sign are on the same side of the river centerline. A value of 0.0 specifies the centerline of the river; the banks of the river channel are at ± one-half the river width. The value specified for the offset distance should not exceed one-half the river width in magnitude.

2047, STREAM VEL

The average uniform velocity of the water flowing in the river channel. For use with the tidal river model, this velocity gives the non-tidal component (i.e., constant outflow stream velocity). The outflow stream velocity can be provided by determining the stream velocity of the river at an upstream point which is not affected by tidal action. Alternatively it can be estimated from the Tidal Current Tables by subtracting the maximum flood current velocity from the maximum ebb current velocity. For conversions, use 1 knot = 51.48 cm/sec.

2048, TIDAL VEL

For spills into a river affected by tidal action, the actual velocity of the flowing water is obtained as the sum of a constant outflow velocity (item 2047) and a sinusoidal component to represent the tidal action. Item 2048 is the maximum amplitude of the tidal current velocity. This data item can be determined by accessing the Tidal Current Tables for the region of interest and by computing the average of the maximum ebb and flood current velocities.

2049, TIDAL PERIOD

For spills into tidal rivers or estuaries, the tidal period is the time from one high tide to the next or from one low tide to the next. The nominal tidal period applicable to most regions is approximately 12 hours.

2050, PHASE LAG

For spills into a tidal river, since the water velocity is represented as the sum of a non-tidal and a tidal component, the time of spill is referenced to the tidal velocity variation by the phase lag. This gives the elapsed time from the start of a spill or discharge to the next high water slack tide (high tide). The phase lag should not exceed the tidal period.

2051, DECAY COEFF

Degradation or decay of a discharged chemical in the

aquatic environment is modeled as a first order exponential decay process (e^{-kt}), and this data item specifies the value of the decay coefficient k. Since the decay reduces the total quantity of dispersing substance, the concentrations are less than if no decay is assumed. Also, dispersion of products of degradation are not modeled, and these may also be hazardous. Conservative estimates of concentrations can be obtained using a value of 0.0.

2052, MANNING FACT

For spills into tidal rivers or estuaries, the Manning factor describes the roughness of the channel bottom and is used in the computation of turbulent dispersion coefficients. By usual convention, the Manning factor is assumed to be non-dimensional; in fact, values are generally tabulated in units of $ft^{1/6}$. To aid in choosing reasonable values, the following table can be used:

Natural-stream Channels	Manning Factor
Clean, straight bank, full stage	0.030
Winding, some pools, and shoals	0.040
Same, but with stony sections	0.055
Sluggish reaches, very deep pools, very weedy	0.070-0.125

4002, TOT MASS LIQ

For either instantaneous or continuous spills, this data item gives the total quantity of liquid which enters the receiving water body.

4049, LIQ FLWRATE

For continuous spills, this item gives the rate at which the liquid chemical enters the receiving water body. The duration of the continuous discharge is determined by the total quantity of discharged liquid (item 4002) divided by the flow rate (item 4049). If the duration of release is known, then the flow rate can be estimated simply by dividing the total mass released by the discharge duration.

2043, DIF COEF H2O

For spills into non-tidal rivers, the model currently obtains an estimate of the turbulent dispersion coefficients using a scaled value of the molecular diffusion coefficient for the discharged chemical in water. The computation of the molecular diffusion coefficient uses a number of physical properties of the spilled chemical which are not otherwise required. The model currently computes an estimate of the turbulent dispersion coefficient for a discharge into still water, then displays this value as a data item which may be changed by the user.

SECTION VII

SAMPLE COMPUTATIONS

Several different spill scenarios are described in this section, and sample outputs from the model execution are included. These illustrate the types of output produced, the sequence of operations performed, and the type of input data required. The sample cases were selected to illustrate outputs for different types of water bodies and spill conditions. A brief narrative is given describing the spill situation, and additional discussion or explanation of the sample output follows. In each case, the sample includes only a single selected model run for the particular case. In actual use, a number of such runs would be made for different conditions, locations, or times relevant to the spill.

1. NON-TIDAL RIVER

Scenario

While loading a tank truck at an on-shore storage facility, a rupture occurs and the entire contents of the tank are released nearly instantaneously. The tank was nearly full, holding about 35,000 pounds of hydrazine when the rupture occurred.

The storage area is close to the shore of a river in which water intake facilities are located about a mile downstream. In this stretch, the river is about 300 feet wide and 30 feet deep, and the current is about 3 miles per hour.

Sample Run

The computer print-out for this sample computation is given in

Figure 3. The spill model is executed using the RUN option; to set up data for a new case, the spill model (P) is specified, and the chemical hydrazine is identified by the three-character recognition code HDZ.

For this run, the default output unit options selection was unchanged. This gives most outputs in CGS units; English units would have been a better choice for the data used in this example.

Property file access was disabled since for this example only the liquid density of the chemical at ambient temperature is needed.

The water body type for a non-tidal river and the instantaneous spill condition were already set as default values so these items were not changed. The liquid density was entered as 1.008 g/cm^3.

The observation point coordinates were entered for the water intake location one mile downstream. It was assumed that the intake is located close to the shore, on the same side of the river as the spill, since the concentrations along this bank will be greater than those near the far bank for some distance downstream from the spill.

Since the river is flowing at 3 MPH, the time required for the spill mass to move 1 mile downstream will be about 20 minutes. At that time, the concentration at the intake will be near to a peak value, so 20 minutes was entered for the time of observation.

River depth and width are entered as 30 feet and 300 feet, respectively. The offset distance is entered as one-half the width, 150 feet, to specify a spill location at the shore; the stream velocity is entered as 3 MPH. Additional information regarding chemical degradation and the channel condition is not available; default values are

Figure 3. Sample Computation for Non-Tidal River

```
          HAZARD ASSESSMENT COMPUTER SYSTEM
          EXECUTION STARTED ON  80/05/16. AT  13.34.18
 ENTER RUN REQUEST, OPTIONS ARE (RUN/RERUN/CONTINUE/END)
? RUN

     HACS STATE FILE INITIALIZED WITH DEFAULT  VALUES, FILE LABEL FOLLOWS -
          HACS DEFAULT FILE - UPDATED 04/30/76 (R. POTTS/J. HAGOPIAN)

 ENTER ASSESSMENT MODEL LETTER CODES (A-Z/II/RR/SS):
? P
      P
 ENTER CHEMICAL RECOGNITION CODE:
? HDZ
 OUTPUT OPTIONS ARE:
   0  SELECT ALL UNITS
   1  SELECT CGS UNITS
   2  SELECT SI UNITS
   3  SELECT ENGLISH UNITS
   4  SELECT MIXED UNITS
     3019 UNIT SELECT   =              1      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
     3002 PLOT OFFLINE  =              0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
     3011 READ PROP     =              1      ND       , IS A  DEFAULT   VALUE
```

Figure 3. Sample Computation for Non-Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 VALUE RANGE IS     0 TO      1
 ENTER INTEGER VALUE:
? 0
     3011 READ PROP      =            0      ND       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
     3018 PROP REPORT    =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 MODEL  P  IS NOW BEING EXECUTED.
 THE INPUTS REQUIRED FOR THIS RATE MODEL ARE...


 WATER BODY OPTIONS ARE:
   1  STILL WATER
   2  NON-TIDAL RIVER
   3  TIDAL RIVER
     2028 WAT TYPE P/R   =            2      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 SPILL TYPE OPTIONS ARE:
   0  INSTANTANEOUS
   1  CONTINUOUS
     2029 SPILL TYPE P   =            0      ND       , IS A  DEFAULT   VALUE
```

Figure 3. Sample Computation for Non-Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
    1004 DENS LIQ AMB  =      .8700      G/CM3    , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /G/CM3   /KG/M3   /LB/FT3  /G/CM3   /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 1.008 G/CM3
    1004 DENS LIQ AMB  =      1.008      G/CM3    , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
    2039 CONC PT X     =      .1000E+06  CM       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM      /M       /FT      /MI      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 1 MI
 INPUT CONVERTED TO UNITS OF CM
 IS     .1609E+06
    2039 CONC PT X     =      .1609E+06  CM       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
    2040 CONC PT Y     =      0.         CM       , IS A  DEFAULT   VALUE
```

Figure 3. Sample Computation for Non-Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM      /M       /FT      /MI      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 150 FT
 INPUT CONVERTED TO UNITS OF CM
 IS     4572.
     2040 CONC PT Y     =      4572.      CM      , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2041 CONC PT Z     =      0.         CM      , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2042 TIME CONC PT  =      600.0      S       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y   ,
 UNITS ARE /S       /S       /MIN     /HR      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 20 MIN
 INPUT CONVERTED TO UNITS OF S
 IS     1200.
     2042 TIME CONC PT  =      1200.      S       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2044 RIVER DEPTH   =      .1000E+05  CM      , IS A  DEFAULT   VALUE
```

Figure 3. Sample Computation for Non-Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM       /M        /FT       /MI       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 30 FT
 INPUT CONVERTED TO UNITS OF CM
 IS      914.4
     2044 RIVER DEPTH    =       914.4       CM       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2045 RIVER WIDTH    =       .1000E+06   CM       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM       /M        /FT       /MI       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 300 FT
 INPUT CONVERTED TO UNITS OF CM
 IS      9144.
     2045 RIVER WIDTH    =       9144.       CM       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2046 OFF DIST       =       0.          CM       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
```

Figure 3. Sample Computation for Non-Tidal River (Continued)

```
 UNITS ARE /CM      /M       /FT      /MI      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 150 FT
 INPUT CONVERTED TO UNITS OF CM
 IS     4572.
     2046 OFF DIST      =      4572.      CM      , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2047 STREAM VEL    =      100.0      CM/S    , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM/S    /M/S     /MPH     /KNOTS   /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 3 MPH
 INPUT CONVERTED TO UNITS OF CM/S
 IS     134.1
     2047 STREAM VEL    =      134.1      CM/S    , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2051 DECAY COEFF   =      0.         /S      , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2052 MANNING FACT  =      .3000E-01  ND      , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
```

Figure 3. Sample Computation for Non-Tidal River (Continued)

```
    4002 TOT MASS LIQ  =      0.          G        , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /G       /KG       /LB       /TN       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 35000 LB
 INPUT CONVERTED TO UNITS OF G
 IS      .1588E+08
     4002 TOT MASS LIQ  =      .1588E+08  G        , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE:
   0  SUPPRESS THIS OUTPUT
   1  CONC. VS TIME AT X,Y,Z
   2  MAXIMUM CONC. VS DISTANCE
   3  BOTH OF THE ABOVE
     3008 PLOT FLAG P   =           0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 VALUE RANGE IS    -1 TO     4
 ENTER INTEGER VALUE:
? 3
     3008 PLOT FLAG P   =           3      ND       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
```

Figure 3. Sample Computation for Non-Tidal River (Continued)

```
     3015 TABLE FLAG P  =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 VALUE RANGE IS    -1 TO    10
 ENTER INTEGER VALUE:
? 3
     3015 TABLE FLAG P  =            3      ND       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2037 MAX TME CONC  =      .3600E+05  S        , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /S       /S       /MIN     /HR      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 2 HR
 INPUT CONVERTED TO UNITS OF S
 IS     7200.
     2037 MAX TME CONC  =      7200.      S        , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 WARNING - MODEL   P  IS USING DEFAULT VALUES
```

Figure 3. Sample Computation for Non-Tidal River (Concluded)

```
THE RESULTS OF MODEL  P  ARE...

    4022 LIQ-H2O CONC  =      .8576E-02  G/CM3    , IS A  COMPUTED  VALUE

THIS CONCENTRATION IS EQUIVALENT TO  8508.     PPM AND  8576.     MG/LITER.

THE EXECUTION OF MODEL  P  IS COMPLETED.
```

used for these items. The quantity of chemical spilled is entered as 35,000 pounds.

Both the plotted and tabular output options are turned on, and the time scale for these outputs is set at 2 hours. Since it was determined above that the concentration at the intake peaks at about 20 minutes, the selected interval will bracket the peak concentration. The plotted output obtained for this sample computation is given in Figure 4. The tabular output produced is given by Tables 2 and 3.

The output shows the actual concentration at the water intake location to be 8508 ppm 20 minutes after the discharge occurs. The passage of the spill mass past the intake is quite rapid, taking only about 0.4 minute. At a current velocity of 3 MPH, this indicates that the width of the dispersing mass is on the order of 100 feet at this distance from the spill location. The second table indicates that concentrations in excess of 1000 ppm will occur for distances up to 5 or 6 miles downstream from the spill. Further runs at successive downstream observation points could be made to correlate arrival times with durations of hazardous concentrations.

2. TIDAL RIVER

Scenario

During the night, a barge, breaking loose, drifts with the current until it collides against a railroad bridge crossing a tidal waterway. Dammage appears to be minimal. However, during the ensuing confusion, an approaching train is unable to stop before entering on the bridge. Two supporting piers, already weakened, shift and the superstructure of the

Figure 4. Concentration Profile for Non-Tidal River Example

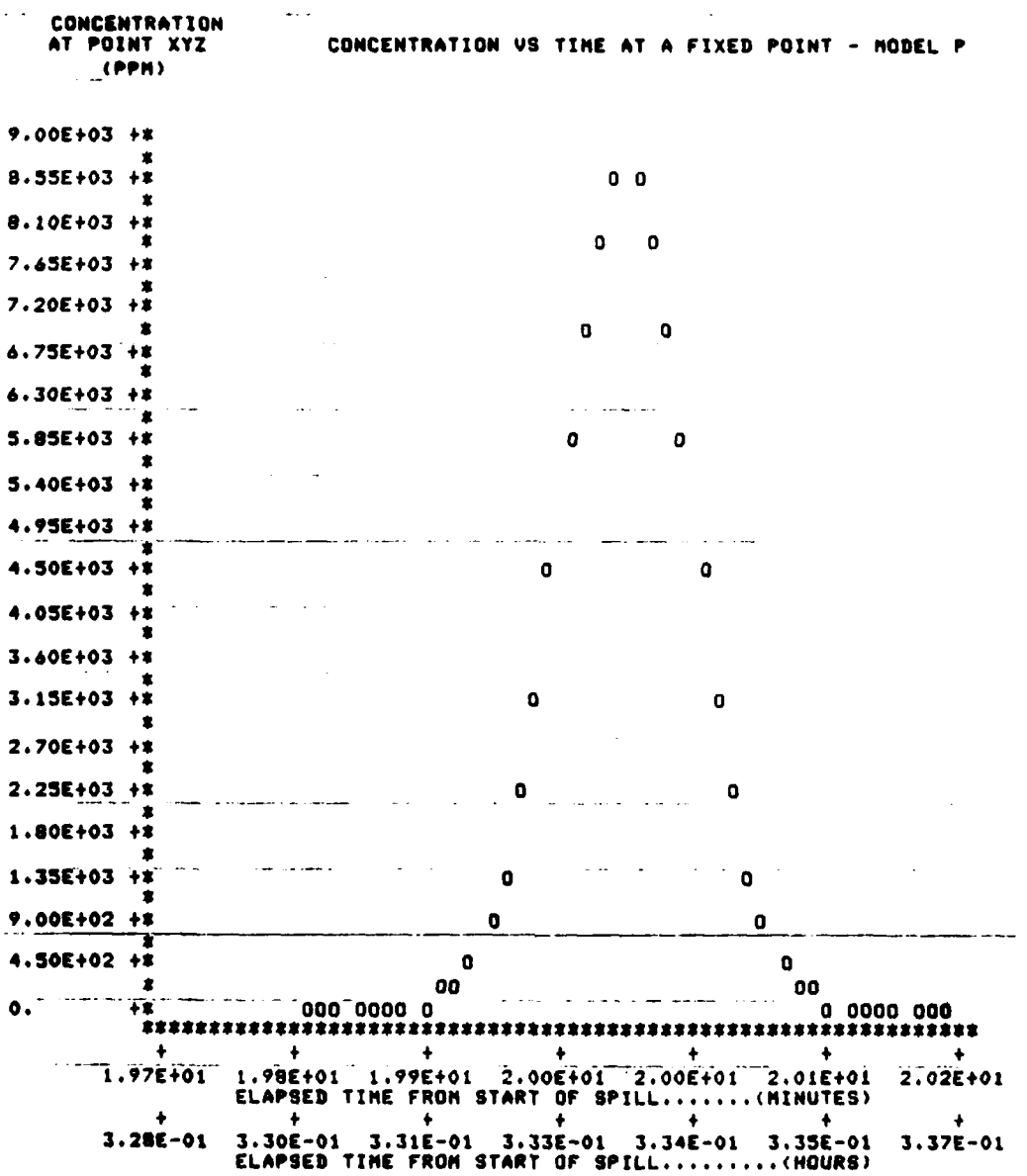
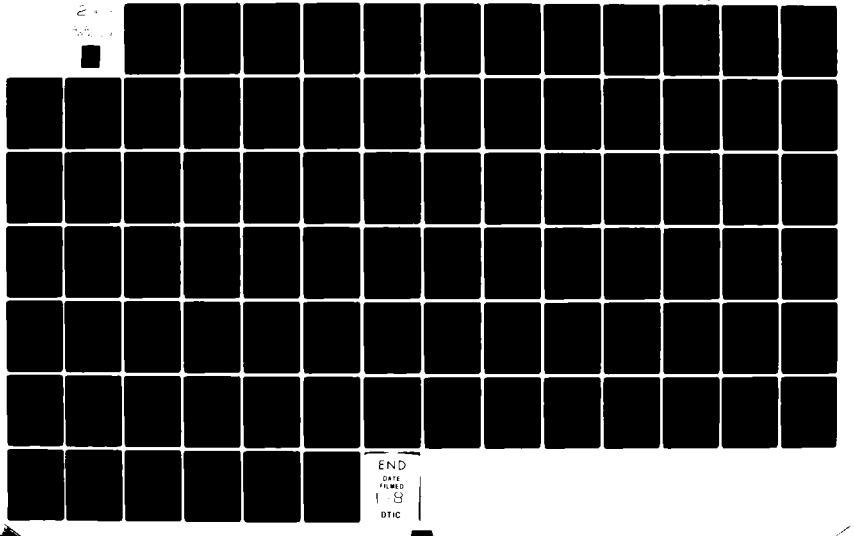


TABLE 2. CONCENTRATION VERSUS TIME FOR NON-TIDAL RIVER EXAMPLE

ELAPSED TIME (MINS)	CONCENTRATION (PPM)	CONCENTRATION (MG/LITER)
19.794	.36342E-01	.36633E-01
19.804	.12585	.12686
19.815	.40785	.41111
19.825	1.2370	1.2469
19.836	3.5118	3.5399
19.846	9.3329	9.4076
19.856	23.221	23.406
19.867	54.094	54.527
19.877	118.00	118.95
19.888	241.06	242.99
19.898	461.24	464.93
19.909	826.64	833.26
19.919	1387.9	1399.0
19.930	2183.1	2200.6
19.940	3217.6	3243.3
19.950	4443.8	4479.3
19.961	5751.7	5797.7
19.971	6977.6	7033.5
19.982	7934.6	7998.1
19.992	8458.6	8526.3
20.003	8454.0	8521.7
20.013	7922.6	7986.0
20.024	6962.4	7018.1
20.034	5738.2	5784.1
20.045	4435.7	4471.2
20.055	3216.4	3242.1
20.065	2187.9	2205.4
20.076	1396.3	1407.5
20.086	836.17	842.86
20.097	469.88	473.64
20.107	247.81	249.79
20.118	122.66	123.64
20.128	56.994	57.450
20.139	24.860	25.059
20.149	10.181	10.262
20.160	3.9147	3.9460
20.170	1.4135	1.4248
20.180	.47934	.48318
20.191	.15267	.15389
20.201	.45675E-01	.46040E-01

AD-A091 803 LITTLE (ARTHUR D) INC CAMBRIDGE MA F/G 13/2
SPILL ASSESSMENT MODEL USER'S MANUAL.(U)
MAY 80 R G POTTS, J H HAGOPIAN F08635-79-C-0084
UNCLASSIFIED AFESC/ESL-TR-80-27 NL



END
DATE FILMED
1 8
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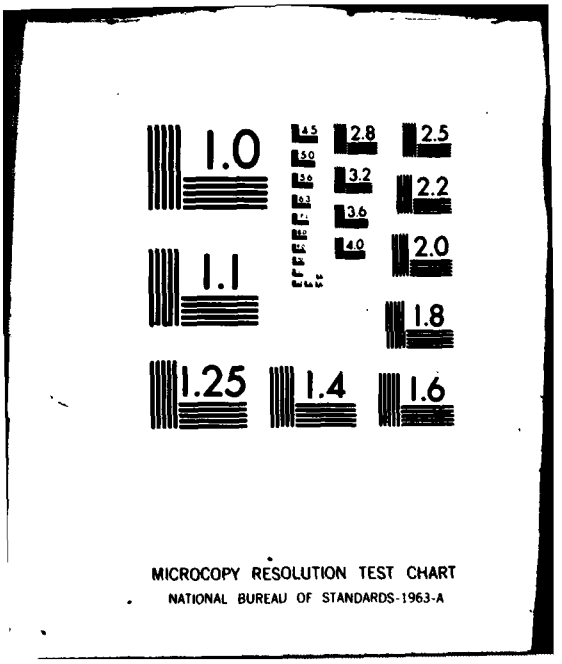
1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0
5.6
6.3
MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

TABLE 3. CONCENTRATION VERSUS TIME AND DISTANCE FOR NON-TIDAL RIVER EXAMPLE

DOWNSTREAM DISTANCE (METERS)	DOWNSTREAM DISTANCE (FEET)	ELAPSED TIME (MINUTES)	CONCENTRATION AT SURFACE (MG/LITER)	CONCENTRATION ON RIVERBED (MG/LITER)
80.46	264.0	1.000	.5352E+06	526.8
326.0	1069.	4.051	.6570E+05	.2003E+05
571.5	1875.	7.103	.2905E+05	.1935E+05
817.0	2680.	10.15	.1819E+05	.1564E+05
1062.	3486.	13.21	.1337E+05	.1259E+05
1308.	4291.	16.26	.1067E+05	.1034E+05
1553.	5097.	19.31	8912.	8685.
1799.	5902.	22.36	7653.	7437.
2045.	6708.	25.41	6697.	6473.
2290.	7513.	28.46	5941.	5711.
2536.	8319.	31.51	5326.	5095.
2781.	9124.	34.56	4815.	4588.
3027.	9930.	37.62	4384.	4164.
3272.	.1074E+05	40.67	4015.	3805.
3518.	.1154E+05	43.72	3696.	3497.
3763.	.1235E+05	46.77	3418.	3230.
4009.	.1315E+05	49.82	3173.	2997.
4254.	.1396E+05	52.87	2957.	2791.
4500.	.1476E+05	55.92	2764.	2609.
4745.	.1557E+05	58.97	2591.	2447.
4991.	.1637E+05	62.03	2436.	2301.
5236.	.1718E+05	65.08	2296.	2169.
5482.	.1798E+05	68.13	2169.	2050.
5727.	.1879E+05	71.18	2053.	1942.
5973.	.1960E+05	74.23	1947.	1843.
6218.	.2040E+05	77.28	1850.	1752.
6464.	.2121E+05	80.33	1761.	1669.
6709.	.2201E+05	83.38	1678.	1592.
6955.	.2282E+05	86.44	1602.	1521.
7200.	.2362E+05	89.49	1532.	1455.
7446.	.2443E+05	92.54	1466.	1394.
7691.	.2523E+05	95.59	1405.	1337.
7937.	.2604E+05	98.64	1349.	1284.
8182.	.2684E+05	101.7	1295.	1234.
8428.	.2765E+05	104.7	1246.	1188.
8673.	.2846E+05	107.8	1199.	1144.
8919.	.2926E+05	110.8	1155.	1103.
9164.	.3007E+05	113.9	1114.	1065.
9410.	.3087E+05	116.9	1076.	1029.
9655.	.3168E+05	120.0	1039.	994.4

NOTE: TABLE GIVES CONCENTRATIONS AT SURFACE AND ON RIVERBED FOR DISTANCES DOWNSTREAM FROM THE SPILL LOCATION. DOWNSTREAM DISTANCE IS GIVEN ALONG LINES ON THE SURFACE AND RIVERBED SHIFTED FROM THE RIVER CENTERLINE BY THE SPILL OFFSET.

bridge begins to collapse. The train comes to rest with a tank car carrying hydrazine at the middle of the span. Damage to the train is extensive, and the tank car appears to have been pierced.

A continuous leak ensues, and it is estimated that the entire tank contents of 50,000 pounds of hydrazine will have entered the waterway after about a one hour duration.

The accident occurs at low tide; the river channel in the area is about 500 feet wide and 45 feet deep. Since the spill occurs as the tide starts to come in, the tidal velocities in the area are relatively large and the tidal period is long. There is concern that hazardous concentrations will exist in the area for an extended duration.

Sample Run

The computer print-out for this sample computation is given in Figure 5. The spill model is executed for hydrazine and the assessment model letter code P. In the case of the sample run, the run request option actually used was CONTINUE, since the sample output actually shown was the second of two runs. In the first run, inputs for the river width and depths were inadvertently transposed. The output of this run shows a majority of the status codes of data items are "USER," indicating items that were previously entered and are now available with the CONTINUE option.

Property file access is again suppressed since only the liquid density is needed. A continuous spill into a tidal river is specified, and the coordinates of the observation point are selected at the spill location. The time of observation is taken as 12 hours, corresponding

Figure 5. Sample Computation for Tidal River

```
 ENTER RUN REQUEST, OPTIONS ARE (RUN/RERUN/CONTINUE/END)
?

  CONTINUE

     HACS STATE FILE INITIALIZED WITH COMPUTED VALUES, FILE LABEL FOLLOWS -


 ENTER ASSESSMENT MODEL LETTER CODES (A-Z/II/RR/SS):
? P
      P
 ENTER CHEMICAL RECOGNITION CODE:
? HDZ
 OUTPUT OPTIONS ARE:
   0  SELECT ALL UNITS
   1  SELECT CGS UNITS
   2  SELECT SI UNITS
   3  SELECT ENGLISH UNITS
   4  SELECT MIXED UNITS
     3019 UNIT SELECT    =            3      ND       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
     3002 PLOT OFFLINE  =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
     3011 READ PROP     =            0      ND       , IS A    USER     VALUE
```

Figure 5. Sample Computation for Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
     3018 PROP REPORT   =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 MODEL  P  IS NOW BEING EXECUTED.
 THE INPUTS REQUIRED FOR THIS RATE MODEL ARE...


 WATER BODY OPTIONS ARE:
   1  STILL WATER
   2  NON-TIDAL RIVER
   3  TIDAL RIVER
     2028 WAT TYPE P/R  =            3      ND       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 SPILL TYPE OPTIONS ARE:
   0  INSTANTANEOUS
   1  CONTINUOUS
     2029 SPILL TYPE P  =            1      ND       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     1004 DENS LIQ AMB  =        62.92      LB/FT3   , IS A    USER    VALUE
```

Figure 5. Sample Computation for Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2039 CONC PT X      =      0.          FT       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2040 CONC PT Y      =      0.          FT       , IS A  DEFAULT    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2041 CONC PT Z      =      0.          FT       , IS A  DEFAULT    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2042 TIME CONC PT   =      720.0       MIN      , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2044 RIVER DEPTH    =      500.0       FT       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM      /M       /FT      /MI      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 45 FT
 INPUT CONVERTED TO UNITS OF CM
 IS     1372.
     2044 RIVER DEPTH    =      45.00       FT       , IS A    USER     VALUE
```

Figure 5. Sample Computation for Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2045 RIVER WIDTH    =       5000.       FT       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM       /M        /FT       /MI       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 500 FT
 INPUT CONVERTED TO UNITS OF CM
 IS      .1524E+05
     2045 RIVER WIDTH    =       500.0       FT       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2046 OFF DIST       =       0.          FT       , IS A  DEFAULT    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2047 STREAM VEL     =       .6905       MPH      , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2048 TIDAL VEL      =       2.762       MPH      , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2049 TIDAL PERIOD   =       1440.       MIN      , IS A    USER     VALUE
```

Figure 5. Sample Computation for Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2050 PHASE LAG     =     0.          MIN     , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /S       /S       /MIN     /HR      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 12 HR
 INPUT CONVERTED TO UNITS OF S
 IS     .4320E+05
     2050 PHASE LAG     =     720.0       MIN     , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2051 DECAY COEFF   =     0.          /MIN    , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2052 MANNING FACT  =     .3000E-01   ND      , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     4002 TOT MASS LIQ  =     .5000E+05   LB      , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     4049 LIQ FLWRATE   =     15.00       LB/S    , IS A    USER    VALUE
```

Figure 5. Sample Computation for Tidal River (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE:
   0  SUPPRESS THIS OUTPUT
   1  CONC. VS TIME AT X,Y,Z
     3008 PLOT FLAG P   =            1      ND       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     3015 TABLE FLAG P  =            1      ND       , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2037 MAX TME CONC  =       2880.       MIN      , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
```

Figure 5. Sample Computation for Tidal River (Concluded)

```
THE RESULTS OF MODEL  P  ARE...

    4022 LIQ-H20 CONC  =      .6350E-05  LB/FT3  , IS A  COMPUTED  VALUE

    *****NOTE - VALUE IN STATE FILE OF     .2013E-42  G/CM3
         IS A COMPUTED VALUE AND WAS NOT REPLACED

THIS CONCENTRATION IS EQUIVALENT TO  .1009     PPM AND  .1017     MG/LITER.

THE EXECUTION OF MODEL  P  IS COMPLETED.
```

to high tide for the area. It is anticipated that, at this time, much of the discharged chemical will actually have moved upstream, and at times greater than 12 hours, the concentrations at the spill location will again increase. Output displays therefore will be scaled over a 48-hour period so that the effects of the tidal action can be observed.

The dimensions of the river channel are entered, and the discharge is assumed to occur at the centerline of the river. Consulting the Tidal Current Tables for the area, the stream velocity (non-tidal component) is determined to be about 0.6 knot and the tidal velocity about 2.4 knots. The tidal period is estimated at about 24 hours, and since the spill started at low tide, the phase lag is entered as 12 hours. Default values are used for both the decay coefficient and the Manning factor.

The total quantity spilled is entered as the capacity of the tank, 50,000 pounds. To enter the discharge rate, a quick calculation arrives at an approximate rate of 15 lb/sec to empty the tank in a one-hour period. The output options were previously set, so no further input is required.

The plotted output obtained for this sample computation is given in Figure 6, and the tabular output is given in Table 4. The model indicates that the concentration at the spill location 12 hours after the spill starts, or 11 hours after the spill stops, is only slightly greater than 0.1 ppm. This elapsed time corresponds to high tide, and as can be seen from the sample plot and table, the concentration at the spill location then rises as the tide goes out. Successive

Figure 6. Concentration Profile for Tidal River Example

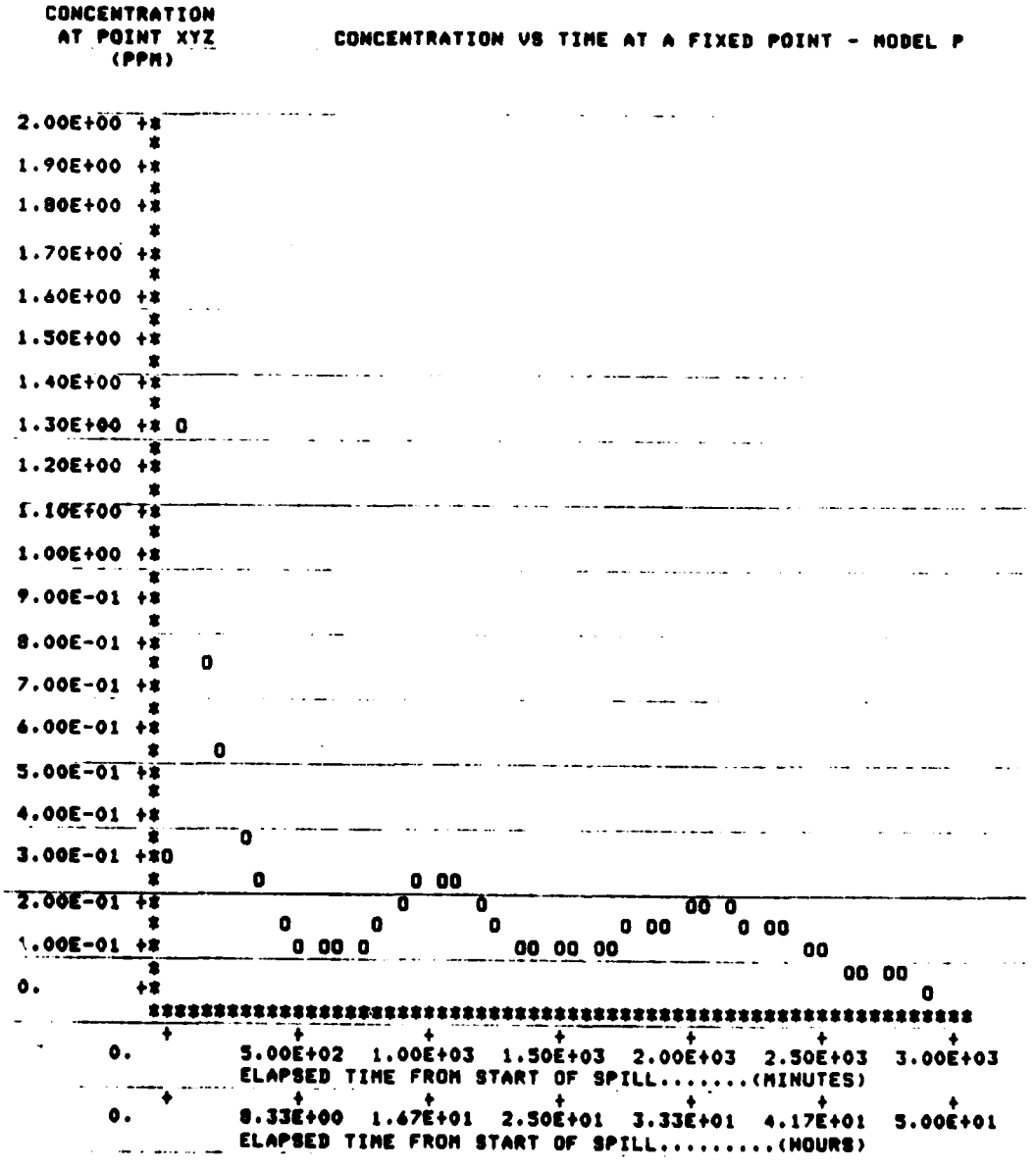

TABLE 4. CONCENTRATION VERSUS TIME FOR TIDAL RIVER EXAMPLE

ELAPSED TIME (MINS)	CONCENTRATION (PPM)	CONCENTRATION (MG/LITER)
1.0000	.29711	.29949
74.821	1.2893	1.2996
148.64	.75596	.76201
222.46	.52997	.53421
296.28	.36131	.36420
370.10	.23694	.23884
443.92	.15420	.15543
517.74	.10868	.10955
591.56	.89619E-01	.90336E-01
665.38	.89722E-01	.90440E-01
739.21	.10720	.10806
813.03	.14298	.14413
886.85	.19348	.19503
960.67	.24165	.24359
1034.5	.26095	.26304
1108.3	.23921	.24112
1182.1	.19194	.19348
1255.9	.14412	.14528
1329.8	.10967	.11054
1403.6	.90502E-01	.91226E-01
1477.4	.84098E-01	.84771E-01
1551.2	.88029E-01	.88733E-01
1625.1	.10062	.10142
1698.9	.11971	.12066
1772.7	.14143	.14256
1846.5	.16066	.16194
1920.3	.17349	.17487
1994.2	.17918	.18061
2068.0	.17955	.18099
2141.8	.17649	.17790
2215.6	.17010	.17146
2289.4	.15865	.15992
2363.3	.14037	.14149
2437.1	.11583	.11676
2510.9	.88875E-01	.89586E-01
2584.7	.64501E-01	.65017E-01
2658.5	.45921E-01	.46288E-01
2732.4	.33654E-01	.33923E-01
2806.2	.26628E-01	.26841E-01
2880.0	.23543E-01	.23731E-01

increases and decreases in concentration take place, corresponding to the tidal action, and successive reduction in value of each peak concentration can be observed.

3. STILL WATER

Scenario

A barge carrying hydrazine across a large lake is involved in a collision. It is estimated that tanks holding approximately 10,000 pounds of hydrazine have been involved, but the quantity of hydrazine remaining in the tanks is not yet known. The water surface is somewhat choppy.

Sample Run

The quantity and duration of release are not completely known, and the spill could be modeled as either an instantaneous release or a continuous release. However, the total quantity discharged cannot be greater than 10,000 pounds. If no further information can be obtained, several assessments should be made assuming an instantaneous release, then assuming a continuous release over several different discharge periods. This sample run illustrates a typical model execution to investigate the instantaneous release condition, actual terminal output is given in Figure 7, with additional explanation in the paragraphs below.

At the start of the execution, the user option to "RUN" is selected for the spill model (P) with the chemical hydrazine, specified by the three-character recognition code HDZ. The output option is selected for English units, and options to retrieve data from the property file (without report) are specified.

Figure 7. Sample Computation for Still Water

```
     HAZARD ASSESSMENT COMPUTER SYSTEM
          EXECUTION STARTED ON  80/05/16. AT  11.46.29
 ENTER RUN REQUEST, OPTIONS ARE (RUN/RERUN/CONTINUE/END)
? RUN

     HACS STATE FILE INITIALIZED WITH DEFAULT  VALUES, FILE LABEL FOLLOWS -
          HACS DEFAULT FILE - UPDATED 04/30/76 (R. POTTS/J. HAGOPIAN)

 ENTER ASSESSMENT MODEL LETTER CODES (A-Z/II/RR/SS):
? P
     P
 ENTER CHEMICAL RECOGNITION CODE:
? HBZ
 OUTPUT OPTIONS ARE:
   0  SELECT ALL UNITS
   1  SELECT CGS UNITS
   2  SELECT SI UNITS
   3  SELECT ENGLISH UNITS
   4  SELECT MIXED UNITS
     3019 UNIT SELECT   =           1     ND      , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 VALUE RANGE IS     0 TO     4
 ENTER INTEGER VALUE:
? 3
     3019 UNIT SELECT   =           3     ND      , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
     3002 PLOT OFFLINE  =           0     ND      , IS A  DEFAULT   VALUE
```

Figure 7. Sample Computation for Still Water (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
    3011 READ PROP     =            1      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 OUTPUT OPTIONS ARE 0=SUPPRESS, 1=SELECT
    3018 PROP REPORT   =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
    STARTING SEARCH OF HACS FILE FOR PHYSICAL PROPERTIES OF CHEMICAL HDZ ...

         FILE OPENED HAS ID = TAPE,  VERSION NUMBER =     1,  DATE =  31877
            BACK-UP FILE ID = NONE,  VERSION NUMBER =     0,  DATE =      0

    PHYSICAL PROPERTY DATA RETRIEVED FOR CHEMICAL HDZ
        NAME = HYDRAZINE
        PATH CODES = A   P   Q
        SHIPPING STATE = L
     1070 HT OF FUSION  =      169.9      BT/LB    , IS A  CHM PROP  VALUE

     *****WARNING - VALUE OF FIELD 1070 HT OF FUSION
          REQUESTED TO BE SAVED EXCEEDS NOMINAL LIMITS OF
              1.200     TO     10.00      CL/G
          SUBSEQUENT CALCULATIONS MAY NOT BE VALID

     2004 TEMP START    =      68.00      F        , IS A  DEFAULT   VALUE
```

Figure 7. Sample Computation for Still Water (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N

     *****WARNING - REQUESTED TEMPERATURE OF      113.6
               IS NOT WITHIN RANGE     5.010      TO      60.01

          COMPUTATION USES TEMPERATURE AT LIMIT OF RANGE


     *****WARNING - REQUESTED TEMPERATURE OF      113.6
               IS NOT WITHIN RANGE    -20.00      TO      100.0

          COMPUTATION USES TEMPERATURE AT LIMIT OF RANGE


     *****WARNING - REQUESTED TEMPERATURE OF      113.6
               IS NOT WITHIN RANGE    0.          TO      50.00

          COMPUTATION USES TEMPERATURE AT LIMIT OF RANGE


     *****WARNING - REQUESTED TEMPERATURE OF      113.6
               IS NOT WITHIN RANGE    0.          TO      30.00

          COMPUTATION USES TEMPERATURE AT LIMIT OF RANGE


     *****WARNING - REQUESTED TEMPERATURE OF      113.6
               IS NOT WITHIN RANGE     1.510      TO      80.01

          COMPUTATION USES TEMPERATURE AT LIMIT OF RANGE

 MODEL  P  IS NOW BEING EXECUTED.
 THE INPUTS REQUIRED FOR THIS RATE MODEL ARE...
```

Figure 7. Sample Computation for Still Water (Continued)

```
 WATER BODY OPTIONS ARE:
   1  STILL WATER
   2  NON-TIDAL RIVER
   3  TIDAL RIVER
     2028 WAT TYPE P/R  =            2      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 VALUE RANGE IS    -1 TO    10
 ENTER INTEGER VALUE:
? 1
     2028 WAT TYPE P/R  =            1      ND       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 SPILL TYPE OPTIONS ARE:
   0  INSTANTANEOUS
   1  CONTINUOUS
     2029 SPILL TYPE P  =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     1002 MOLEC WEIGHT  =       32.05       LB/LBM   , IS A  CHM PROP  VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     1003 BOIL TEM LIQ  =       236.4       F        , IS A  CHM PROP  VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
```

Figure 7. Sample Computation for Still Water (Continued)

```
     1004 DENS LIQ AMB  =       62.90       LB/FT3   , IS A
!!!!!!  VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):!
? N
     1021 LIQ DENS BP   =       60.72       LB/FT3   , IS A  ESTIMATE  VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):!
? N
     1025 CRIT TEMP     =       715.7       F        , IS A  CHM PROP  VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):!
? N
     2023 WATER TEMP    =       59.00       F        , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):!
? Y
 UNITS ARE /C       /K       /F       /K       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:!
? 68. F
 INPUT CONVERTED TO UNITS OF C
 IS     20.00
     2023 WATER TEMP    =       68.00       F        , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):!
? N
     2039 CONC PT X     =       3281.       FT       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):!
? Y
```

Figure 7. Sample Computation for Still Water (Continued)

```
 UNITS ARE /CM       /M        /FT       /MI       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 100 FT
 INPUT CONVERTED TO UNITS OF CM
 IS      3048.
     2039 CONC PT X      =       100.0       FT       , IS A    USER     VALUE
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2040 CONC PT Y      =       0.          FT       , IS A  DEFAULT    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2041 CONC PT Z      =       0.          FT       , IS A  DEFAULT    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2042 TIME CONC PT   =       10.00       MIN      , IS A  DEFAULT    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /S        /S        /MIN      /HR       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 48 HR
 INPUT CONVERTED TO UNITS OF S
 IS       .1728E+06
     2042 TIME CONC PT   =       2880.       MIN      , IS A    USER     VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2051 DECAY COEFF    =       0.          /MIN     , IS A  DEFAULT    VALUE
```

Figure 7. Sample Computation for Still Water (Continued)

```
 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     4002 TOT MASS LIQ  =      0.          LB       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /G       /KG      /LB      /TN      /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 10000 LB
 INPUT CONVERTED TO UNITS OF G
 IS      .4536E+07
     4002 TOT MASS LIQ  =      .1000E+05  LB       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N

 THE DIFFUSION COEFFICIENT OF THE CHEMICAL IN WATER IS CALCULATED

     2043 DIF COEF H2O  =      .1841E-04  FT2/S    , IS A  COMPUTED  VALUE

     2043 DIF COEF H2O  =      .1841E-04  FT2/S    , IS A  COMPUTED  VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 UNITS ARE /CM2/S   /M2/S    /FT2/S   /M2/S    /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 100. CM2/S
     2043 DIF COEF H2O  =      .1076      FT2/S    , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
```

Figure 7. Sample Computation for Still Water (Continued)

```
 OUTPUT OPTIONS ARE:
   0  SUPPRESS THIS OUTPUT
   1  CONC. VS TIME AT X,Y,Z
     3008 PLOT FLAG P   =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 VALUE RANGE IS    -1 TO     4
 ENTER INTEGER VALUE:
? 1
     3008 PLOT FLAG P   =            1      ND       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     3015 TABLE FLAG P  =            0      ND       , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? Y
 VALUE RANGE IS    -1 TO    10
 ENTER INTEGER VALUE:
? 1
     3015 TABLE FLAG P  =            1      ND       , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
     2037 MAX TME CONC  =       600.0       MIN      , IS A  DEFAULT   VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
```

Figure 7. Sample Computation for Still Water (Concluded)

```
? Y
 UNITS ARE /S        /S        /MIN      /HR       /
 ENTER DECIMAL VALUE AND OPTIONAL UNIT LABEL:
? 24 HR
 INPUT CONVERTED TO UNITS OF S
 IS      .8640E+05
     2037 MAX THE CONC  =       1440.       MIN      , IS A    USER    VALUE

 DO YOU WANT TO CHANGE THIS INPUT VALUE?
 ENTER YES OR NO (Y/N):
? N
 WARNING - MODEL   P  IS USING DEFAULT VALUES
```



```
THE RESULTS OF MODEL  P  ARE...

    4022 LIQ-H20 CONC  =       .1547E-03  LB/FT3  , IS A  COMPUTED  VALUE


    THIS CONCENTRATION IS EQUIVALENT TO  2.460     PPM AND  2.479     MG/LITER.

    THE EXECUTION OF MODEL  P  IS COMPLETED.
```

The physical property data for hydrazine is retrieved and stored in the model. Warning messages are printed because properties which are functions of temperature are being computed at a temperature beyond the range of the data given for hydrazine. The actual values stored, except for liquid density, are not required by this model, and the warning diagnostics are ignored.

The execution of the spill model starts by entering input data to select the still water (lake) case and an instantaneous spill.

Chemical property data stored in the model is left unchanged. The display of water temperature shows the value currently at 59°F, a default which is different than the starting temperature used earlier. This data item is changed to 68°F, although there is no confirmation that this agrees with on-scene conditions.

The coordinates of the observation point are taken at the surface of the water, at a point located 100 feet from the spill. Further runs would use different coordinates to evaluate the characteristics of the dispersion of the spilled chemical. The time the concentration is to be obtained is set at 48 hours after the spill occurs. A conservative assumption is made by leaving the decay coefficient at its default setting of zero. The quantity of spilled chemical is entered as 10,000 pounds. Since the surface of the water body has been reported as choppy, the computed value of the dispersion coefficient based on scaled molecular diffusion is replaced by a user value of 100 cm^2/sec. Finally the output options are turned on and scaled to report results for the first 24-hour period following the spill. Output produced from this run is given in Figure 8 and Table 5.

Figure 8. Concentration Profile for Still Water Example

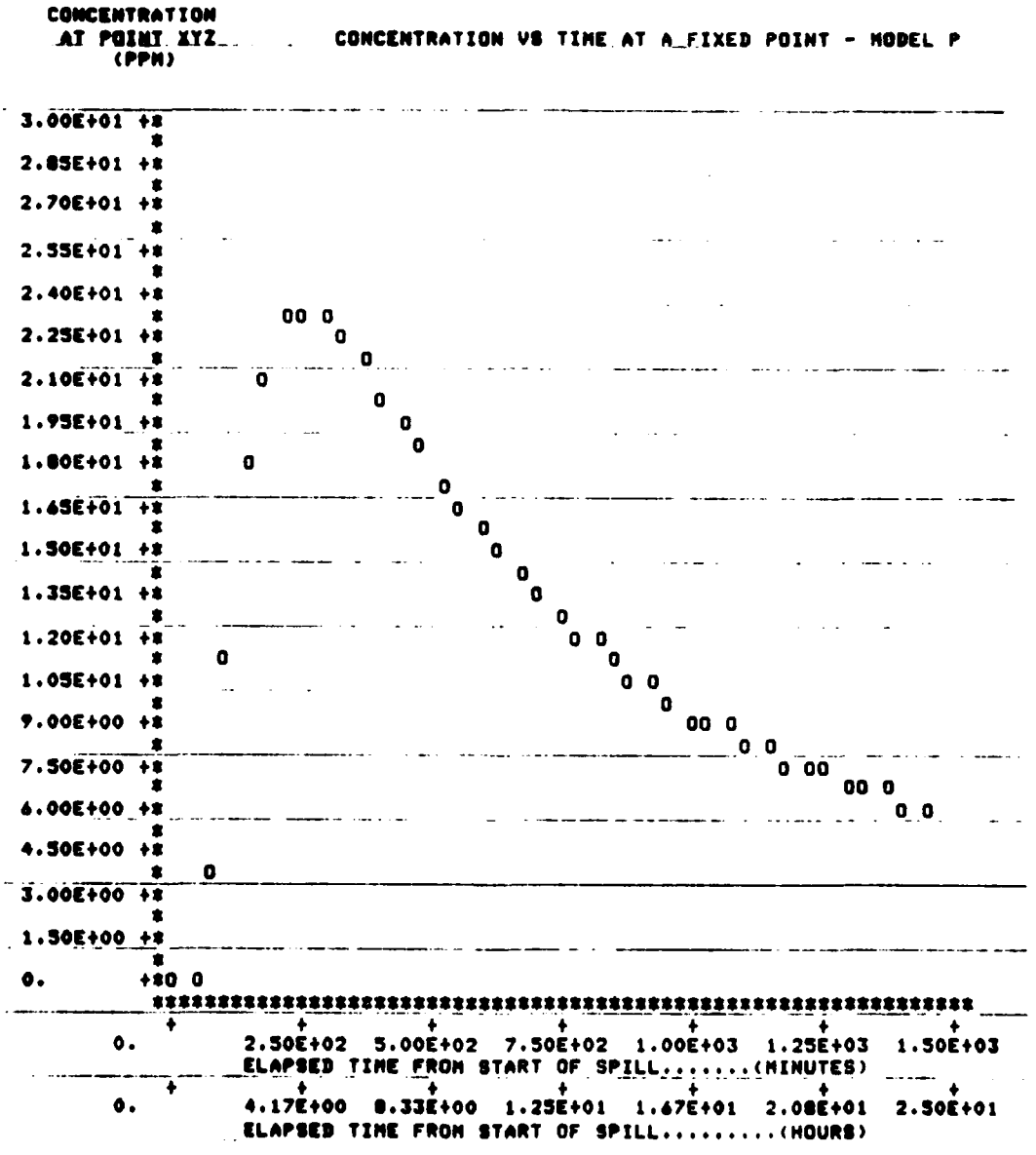

TABLE 5. CONCENTRATION VERSUS TIME FOR STILL WATER EXAMPLE

ELAPSED TIME (MINS)	CONCENTRATION (PPM)	CONCENTRATION (MG/LITER)
1.0000	.33474-162	.33729-162
37.897	.68303E-01	.68822E-01
74.795	3.8010	3.8299
111.69	11.513	11.600
148.59	17.742	17.877
185.49	21.358	21.521
222.38	23.001	23.176
259.28	23.406	23.584
296.18	23.090	23.266
333.08	22.378	22.548
369.97	21.464	21.628
406.87	20.464	20.620
443.77	19.445	19.593
480.67	18.444	18.584
517.56	17.483	17.616
554.46	16.571	16.698
591.36	15.715	15.834
628.26	14.913	15.027
665.15	14.166	14.274
702.05	13.470	13.572
738.95	12.822	12.919
775.85	12.219	12.312
812.74	11.657	11.746
849.64	11.134	11.219
886.54	10.646	10.727
923.44	10.191	10.268
960.33	9.7651	9.8394
997.23	9.3669	9.4382
1034.1	8.9938	9.0622
1071.0	8.6438	8.7096
1107.9	8.3151	8.3784
1144.8	8.0060	8.0669
1181.7	7.7150	7.7737
1218.6	7.4407	7.4973
1255.5	7.1819	7.2365
1292.4	6.9373	6.9901
1329.3	6.7060	6.7570
1366.2	6.4870	6.5364
1403.1	6.2794	6.3272
1440.0	6.0825	6.1288

The computed concentration at the observation point, 100 feet away from the spill, shows that the concentration is reduced to 2.46 ppm after 48 hours from the spill. The printed and plotted display shows that the peak concentration at this point is approximately 23.4 ppm and that this is reached at about 4 hours after the start of the spill. A concentration of 10 ppm exists at this location for approximately 13 hours, and this concentration is reached at about 2 hours after the spill occurs. Concentrations are not reduced to below 10 ppm at this location until about 15 hours after the spill.

After the requested table is printed, the user may enter new observation point coordinates and obtain different sets of plots and tables or re-run the model for different assumptions (e.g., continuous release).

SECTION VIII

REVIEW OF MAJOR ASSUMPTIONS

Because of the complexity of the chemical spill process, the uncertainties and variabilities associated with spill conditions and the nature of the environment in the vicinity of the spill, and the difficulties inherent in describing these phenomena, the analysis and implementation of the water dispersion model has necessarily been based on numerous assumptions. The degree of sophistication that has been attempted has been carefully considered, and assumptions or limitations introduced to enable the models to be applied to a class of non-chemical specific discharges in a range of environmental settings. Also, these models are intended for use in real or threatened emergency spill situations, in addition to routine assessments for contingency planning, and thus the input data required is restricted to that information that can be readily observed, estimated, or assumed from on scene observations or reports; use of extensive, detailed site specific data is precluded. Major assumptions and/or limitations that are incorporated in the model are summarized for review in the following paragraphs.

Heat sources and heat sinks are neglected, and the assumption is made that the initial temperature of the spilled chemical and the receiving water body are nearly equal. Any initial unequal temperatures would ultimately come to equilibrium at a temperature very nearly equal to the temperature of the water into which the spill occurs because of the comparatively large thermal capacity of a river, lake, or ocean into which a spill may

occur. During the initial stages of dispersion, the difference in the temperatures of the spilled chemical and the receiving water could affect the rate of dispersion. The significance of this assumption depends on the type of chemical and relative temperature ranges at which these are transported.

Temperature differences may also give rise to buoyancy effects. Studies of these effects have been reported in the literature, many of them dealing with thermal discharges from power plants or waste water discharges through submerged outlets or distributed outfalls. In these cases, the discharge is lighter than the receiving water. The movement of the discharge as it rises creates secondary induced turbulent currents and the rate of dispersion and manner in which it takes place are effected. The spill model assumes that the spill occurs onto the surface of the waterway, and the effect of buoyancy has not been incorporated. Thus, the model strictly is most appropriate for those liquids that are neither significantly lighter nor denser than the receiving water. The model may also be applied for the dispersion of solid particles, if these are neutrally buoyant or if the settling times are large in comparison to the dispersion.

Chemical degradation in the aquatic environment has been modeled by a first order rate constant process. Additional effects of chemical reactions or phase changes during dispersion have not been incorporated. Phenomena associated with chemical reactions, and also neglected, include resulting dispersion of the products of reaction, and thermal effects from the heat of reaction. The most significant model assumption may be that no vapor is liberated, and that other than a first order decay, the entire mass of spilled chemical is dispersed. The model assumes the chemical is fully

soluble in water (miscible in all proportions) and that all the discharged chemical goes into solution with water. A separate model has been developed for use in HACS to estimate vaporization rates; however, the resulting reduction of the mass dispersing in water has not been incorporated. This assumption leads to estimates of concentrations in water that are conservative.

Stratification of the receiving water body and the interaction with density or buoyancy effects have not been included, although the receiving water body is considered to be non-isotropic, with different but constant dispersion coefficients along each axis. Thermal layers in lakes and oceans are known to exist at some depths, at some or all different times of the year, depending on seasonal temperature variations. These horizontal layers, when present, can act as confining boundaries by significantly inhibiting dispersion to greater depths, reflecting the dispersing chemical and limiting mixing to occur in the upper portion of the water body. Modification of the still water model to incorporate confining boundaries, using the method of imaging or virtual sources, would not present significant difficulty, provided that depths to these boundaries could be estimated.

Strictly, the models apply to spills of large quantities that occur under assumed instantaneous or continuous discharge conditions. For continuous discharges, the rate at which the chemical is released is assumed to be constant. An analysis of the continuous release model has formulated an approach in which a variable mass release rate can be modeled. However, as implemented, the model is limited to a constant release rate since for the purpose of expected use it was assumed that inadequate information would be available to accurately characterize a variable rate.

River channels are modeled as having a constant rectangular cross section, and for non-tidal rivers, a constant cross-sectional average river velocity has been assumed. For tidal rivers, the tidal effect has been modeled by a sinusoidal velocity imposed on the non-tidal component. Velocity variations caused by winds, storms, local channel obstructions, and similar effects have not been included. The boundaries (banks and channel bottom) of the river channel have been assumed to be impenetrable to the dispersing mass, and only first order image sources have been included to model the effect of confined dispersion.

In regions near to the source for a continuous discharge into a river, the additional longitudinal travel due to longitudinal dispersion is neglected with respect to the bulk motion of the dispersing mass in the direction of river travel. This assumption is strictly applicable to rivers in which the rate of longitudinal diffusion is small with respect to the movement with the river velocity; however, all but the most slowly flowing rivers will give reasonably good agreement with this assumption.

At distances far from the location of a spill into a non-tidal river, a simplifying assumption is made that the dispersing mass reaches a uniform cross-sectional distribution, and further dispersion occurs in a one-dimensional manner in the direction of river flow. While the assumption is reasonably consistent with the expected behavior of the mass at large distances from the spill and introduces some simplicity in the model formulation, the resulting difference in the modeling equations may cause a discontinuity in concentration estimates between the near-field and far-field regions. Since the model incorporates, to a first order, the boundary effects in the region near the spill site, concentrations reached at long distances

from the spill location should be expected to approximate those obtained by one-dimensional analysis, and as a result the one-dimensional analysis is not essential. The model does not currently include provision for automatically forcing a match between these near- and far-field equations, and the results obtained should instead be interpreted in terms of the type of dispersion being modeled.

Although some of these assumptions and limitations have greater effect than others, it is generally concluded that the assumptions lead to a simplified, but reasonably realistic, model with which estimates of concentration distributions can be obtained on the same order of accuracy as the accuracy to which the required model inputs are available.

APPENDIX A

INDEX OF CHEMICAL RECOGNITION CODES

This appendix reproduces the full set of 900 chemical recognition codes (Table A-1) for the chemicals contained in the Hazardous Chemical Data Manual of the Chemical Hazard Response Information System, published by the U.S. Coast Guard in October 1978.

The index is in alphabetical order by three-character recognition code and gives the recognition code and compound name for each substance.

Retrieval of physical property data within the Hazard Assessment Computer System is obtained by specifying the three-character chemical recognition code.

TABLE A-1. INDEX OF CODES

AAC	ACETIC ACID
AAD	ACETALDEHYDE
AAM	ACRYLAMIDE
AAN	n-AMYL ALCOHOL
AAT	AMMONIUM ACETATE
ABC	AMMONIUM BICARBONATE
ABF	AMMONIUM BIFLUORIDE
ABM	ACETYL BROMIDE
ABR	ALLYL BROMIDE
ABS	ALKYLBENZENESULFONIC ACIDS
ABZ	AMMONIUM BENZOATE
ACA	ACETIC ANHYDRIDE
ACB	AMMONIUM CARBONATE
ACC	ACETYL CHLORIDE
ACD	ACRIDINE
ACE	ACETYLENE
ACF	ALLYL CHLOROFORMATE
ACI	AMMONIUM CITRATE
ACL	ALUMINUM CHLORIDE
ACN	ACRYLONITRILE
ACP	ACETOPHENONE
ACR	ACRYLIC ACID
ACT	ACETONE
ACY	ACETONE CYANOHYDRIN
ADA	ADIPIC ACID
ADN	ADIPONITRILE
AEA	AMINOETHANOLAMINE
AFM	AMMONIUM FORMATE
AFR	AMMONIUM FLUORIDE
AGC	AMMONIUM GLUCONATE
AID	AMMONIUM IODIDE
ALA	ALLYL ALCOHOL
ALC	ALLYL CHLORIDE
ALD	ALDRIN
ALF	ALUMINUM FLUORIDE

TABLE A-1. INDEX OF CODES (CONTINUED)

ALM	ALUMINUM SULFATE
ALN	ALUMINUM NITRATE
ALS	AMMONIUM LAURYL SULFATE
ALT	AMMONIUM LACTATE
AMA	AMMONIA, ANHYDROUS
AMB	AMMONIUM MOLYBDATE
AMC	AMMONIUM CHLORIDE
AMD	AMMONIUM DICHROMATE
AMF	AMMONIUM SULFITE
AMH	AMMONIUM HYDROXIDE (<28% AQUEOUS AMMONIA)
AMK	n-AMYL METHYL KETONE
AML	AMYL ACETATE
AMM	n-AMYL MERCAPTAN
AMN	AMMONIUM NITRATE
AMP	AMMONIUM PERCHLORATE
AMR	AMMONIUM STEARATE
AMS	AMMONIUM SULFATE
AMT	AMMONIUM THIOCYANATE
AMY	n-AMYL CHLORIDE
AMI	iso-AMYL NITRITE
ANL	ANILINE
ANP	AMMONIUM NITRATE - PHOSPHATE MIXTURE
ANS	AMMONIUM NITRATE - SULFATE MIXTURE
ANT	n-AMYL NITRATE
ANU	AMMONIUM NITRATE—UREA SOLUTION
AOL	AMMONIUM OLEATE
AOX	AMMONIUM OXALATE
APB	AMMONIUM PENTABORATE
APC	ANTIMONY PENTACHLORIDE
APE	AMMONIUM PERSULFATE
APF	ANTIMONY PENTAFLUORIDE
APP	AMMONIUM PHOSPHATE
APS	ACETYL PEROXIDE SOLUTION
APT	ANTIMONY POTASSIUM TARTRATE

TABLE A-1. INDEX OF CODES (CONTINUED)

ARD	ARSENIC DISULFIDE
ARF	ASPHALT BLENDING STOCKS: ROOFERS FLUX
ARL	ACROLEIN
ART	ARSENIC TRISULFIDE
ASA	ARSENIC ACID
ASC	ANISOYL CHLORIDE
ASF	AMMONIUM SULFIDE
ASL	AMMONIUM SILICOFLUORIDE
ASM	AMMONIUM SULFAMATE
ASP	ASPHALT
ASR	ASPHALT BLENDING STOCKS: STRAIGHT RUN RESIDUE
AST	ARSENIC TRICHLORIDE
ATA	ACETYLACETONE
ATC	ALLYLTRICHLOROSILANE
ATF	AMMONIUM THIOSULFATE
ATH	ANTHRACENE
ATM	ANTIMONY TRICHLORIDE
ATN	ACETONITRILE
ATO	ARSENIC TRIOXIDE
ATR	AMMONIUM TARTRATE
ATS	n-AMYLTRICHLOROSILANE
ATT	ANTIMONY TRIFLUORIDE
ATX	ANTIMONY TRIOXIDE
ATZ	ATRAZINE
AZM	AZINPHOSMETHYL
BAC	BORIC ACID
BAD	iso-BUTYRALDEHYDE
BAI	iso-BUTYL ACRYLATE
BAL	BENZYL ALCOHOL
BAM	n-BUTYLAMINE
BAN	n-BUTYL ALCOHOL
BAS	sec-BUTYL ALCOHOL
BAT	tert-BUTYL ALCOHOL

TABLE A-1. INDEX OF CODES (CONTINUED)

BBP	BENZYL n-BUTYL PHTHALATE
BBR	BENZYL BROMIDE
BBZ	BROMOBENZENE
BCF	BENZYL CHLOROFORMATE
BCL	BENZYL CHLORIDE
BCM	n-BUTYL ACETATE
BCP	BOILER COMPOUND, LIQUID
BCR	BARIUM CHLORATE
BCS	BUTYLTRICHLOROSILANE
BDE	BISPHENOL A DIGLYCIDYL ETHER
BDI	BUTADIENE, INHIBITED
BDO	1,4-BUTANEDIOL
BEC	BERYLLIUM CHLORIDE
BEF	BERYLLIUM FLUORIDE
BEM	BERYLLIUM, METALLIC
BEN	BERYLLIUM NITRATE
BEO	BERYLLIUM OXIDE
BES	BERYLLIUM SULFATE
BHC	BENZENE HEXACHLORIDE
BHP	tert-BUTYL HYDROPEROXIDE
BMA	BENZYLTRIMETHYLAMMONIUM CHLORIDE
BMS	n-BUTYL METHACRYLATE
BNT	BARIUM NITRATE
BNZ	BENZENE
BOC	BISMUTH OXYCHLORIDE
BPA	BISPHENOL A
BPC	BARIUM PERCHLORATE
BPD	BENZENE PHOSPHORUS DICHLORIDE
BPF	BROMINE PENTAFLUORIDE
BPM	BARIUM PERMANGANATE
BPO	BARIUM PEROXIDE
BPT	BENZENE PHOSPHORUS THIODICHLORIDE
BRA	n-BUTYRIC ACID
BRC	BARIUM CARBONATE
BRT	BORON TRICHLORIDE

TABLE A-1. INDEX OF CODES (CONTINUED)

BRU	BRUCINE
BRX	BROMINE
BTA	sec-BUTYL ACETATE
BTB	BORON TRIBROMIDE
BTC	n-BUTYL ACRYLATE
BTD	1,4-BUTYNEDIOL
BTF	BROMINE TRIFLUORIDE
BTL	sec-BUTYLAMINE
BTM	n-BUTYL MERCAPTAN
BTN	BUTYLENE
BTO	BUTYLENE OXIDE
BTP	p-tert-BUTYLPHENOL
BTR	n-BUTYRALDEHYDE
BUA	tert-BUTYLAMINE
BUD	1,4-BUTENEDIOL
BUT	BUTANE
BZA	BENZOIC ACID
BZC	BENZOYL CHLORIDE
BZD	BENZALDEHYDE
BZM	BENZYLAMINE
BZN	BENZONITRILE
BZO	BENZYLDIMETHYLOCTADECYLAMMONIUM CHLORIDE
BZP	BENZOPHENONE
CAA	COPPER ACETOARSENITE
CAC	CHLOROACETYL CHLORIDE
CAF	CALCIUM FLUORIDE
CAH	CALCIUM HYDROXIDE
CAL	CALCIUM PHOSPHATE
CAM	CALCIUM, METALLIC
CAO	CALCIUM OXIDE
CAP	p-CHLOROANILINE
CAR	CARENE
CAT	CADMIUM ACETATE
CBA	COBALT ACETATE

TABLE A-1. INDEX OF CODES (CONTINUED)

CBB	CARBON BISULFIDE
CBC	COBALT CHLORIDE
CBN	4-CHLOROBUTYRONITRILE
CBO	CARBOLIC OIL
CBR	CYANOGEN BROMIDE
CBS	COBALT SULFATE
CBT	CARBON TETRACHLORIDE
CBY	CARBARYL
CCA	CALCIUM ARSENATE
CCB	CALCIUM CARBIDE
CCC	CALCIUM CHLORATE
CCH	CYCLOHEXANONE
CCL	CYANOGEN CHLORIDE
CCN	CALCIUM CYANIDE
CCP	CALCIUM PEROXIDE
CCR	CALCIUM CHROMATE
CCT	CREOSOTE, COAL TAR
CCY	COPPER CYANIDE
CDA	CACODYLIC ACID
CDC	CADMIUM CHLORIDE
CDN	CHLORDANE
CDO	CARBON DIOXIDE
CES	CUPRIETHYLENEDIAMINE SOLUTION
CFB	CADMIUM FLUOROBORATE
CGE	CRESYL GLYCIDYL ETHER
CHA	CYCLOHEXYLAMINE
CHC	CHARCOAL
CHD	CHLOROHYDRINS (CRUDE)
CHN	CYCLOHEXANOL
CHP	CYCLOHEXANONE PEROXIDE
CHT	CYCLOHEXENYLTRICHLOROSILANE
CHX	CYCLOHEXANE
CHY	CALCIUM HYPOCHLORITE

TABLE A-1. INDEX OF CODES (CONTINUED)

CID	COPPER IODIDE
CIT	CITRIC ACID
CLC	CALCIUM CHLORIDE
CLD	COLLODION
CLS	CAPROLACTAM, SOLUTION
CLX	CHLORINE
CMA	CHROMIC ANHYDRIDE
CMB	CADMIUM BROMIDE
CMC	CHROMYL CHLORIDE
CME	CHLOROMETHYL METHYL ETHER
CMH	CUMENE HYDROPEROXIDE
CMN	CADMIUM NITRATE
CMO	CARBON MONOXIDE
CMP	p-CYMENE
CMS	CADMIUM SULFATE
CNI	COPPER NITRATE
CNN	COPPER NAPHTHENATE
CNT	CALCIUM NITRATE
COL	COPPER OXALATE
CON	COBALT NITRATE
COP	COPPER ACETATE
COU	COUMAPHOS
COX	CADMIUM OXIDE
CPA	COPPER ARSENITE
CPB	COPPER BROMIDE
CPC	COPPER CHLORIDE
CPF	COPPER FLUOROBORATE
CPH	CAMPHENE
CPL	CHLOROPICRIN, LIQUID
CPN	p-CHLOROPHENOL
CPO	CAMPHOR OIL
CPP	CALCIUM PHOSPHIDE
CPR	CYCLOPROPANE
CPS	CAUSTIC POTASH SOLUTION
CPT	CAPTAN

TABLE A-1. INDEX OF CODES (CONTINUED)

CBA	CHLOROACETOPHENONE
CRB	CHLOROBENZENE
CRE	CALCIUM RESINATE
CRF	CHLOROFORM
CRS	CRESOLS
CSA	CHLOROSULFONIC ACID
CSF	COPPER SULFATE
CSS	CAUSTIC SODA SOLUTION
CSY	CORN SYRUP
CTA	CROTONALDEHYDE
CTC	CATECHOL
CTD	4-CHLORO-o-TOLUIDINE
CTF	CHLORINE TRIFLUORIDE
CUM	CUMENE
CYA	CYANOACETIC ACID
CYG	CYANOGEN
CYP	CYCLOPENTANE
DAA	DIACETONE ALCOHOL
DAC	DIMETHYLACETAMIDE
DAI	DODECYLBENZENESULFONIC ACID, ISOPROPYLAMINE SALT
DAL	DECALDEHYDE
DAM	DIPHENYLAMINE
DAN	n-DECYL ALCOHOL
DAP	DI-n-AMYL PHTHALATE
DBA	DI-n-BUTYLAMINE
DBC	DIISOBUTYLCARBINOL
DBE	DI-n-BUTYL ETHER
DBK	DI-n-BUTYL KETONE
DBL	DIISOBUTYLENE
DBO	o-DICHLOROBENZENE
DBP	p-DICHLOROBENZENE
DBR	DECABORANE
DBS	DODECYLBENZENESULFONIC ACID, TRIETHANOLAMINE SALT

TABLE A-1. INDEX OF CODES (CONTINUED)

DBT	DIBUTYLPHENOL
DBZ	n-DECYLBENZENE
DCA	2,4-DICHLOROPHENOXYACETIC ACID
DCB	DICHLOROBUTENE
DCE	1-DECENE
DCF	DICHLORODIFLUOROMETHANE
DCM	DICHLOROMETHANE
DCP	2,4-DICHLOROPHENOL
DCS	DODECYLBENZENESULFONIC ACID, CALCIUM SALT
DDB	DODECYLBENZENE
DDC	1-DODECENE
DDD	D D D
DDN	DODECANOL
DDS	DODECYL SULFATE, SODIUM SALT
DDT	DDT
DDW	DIMETHYLHEXANE DIHYDROPEROXIDE, WET
DEA	DIETHANOLAMINE
DEB	DIETHYLBENZENE
DEC	DIETHYL CARBONATE
DED	DIELDRIN
DEE	DICHLOROETHYL ETHER
DEG	DIETHYLENE GLYCOL
DEL	1,2-DICHLOROETHYLENE
DEM	DIETHYLENEGLYCOL MONOBUTYL ETHER ACETATE
DEN	DIETHYLAMINE
DEP	DI-(2-ETHYLHEXYL)PHOSPHORIC ACID
DES	2,4-D ESTERS
DET	DIETHYLENETRIAMINE
DEZ	DIETHYLZINC
DFA	DIFLUOROPHOSPHORIC ACID, ANHYDROUS
DFE	1,1-DIFLUOROETHANE
DFF	DISTILLATES: FLASHED FEED STOCKS
DGD	DIETHYLENE GLYCOL DIMETHYL ETHER
DGE	DIETHYLENE GLYCOL MONOETHYL ETHER

TABLE A-1. INDEX OF CODES (CONTINUED)

DGM	DIETHYLENE GLYCOL MONOMETHYL ETHER
DHN	DECAHYDRONAPHTHALENE
DHP	DIHEPTYL PHTHALATE
DIA	DIISOPROPYLAMINE
DID	DIISODECYL PHTHALATE
DIH	DIISOPROPYLBENZENE HYDROPEROXIDE
DIK	DIISOBUTYL KETONE
DIM	DIMETHYL ETHER
DIP	DIISOPROPANOLAMINE
DLP	DALAPON
DMA	DIMETHYLAMINE
DMD	DIMETHYLDICHLOROSILANE
DME	DIETHYLENEGLYCOL MONOBUTYL ETHER
DMF	DIMETHYLFORMAMIDE
DMH	1,1-DIMETHYLHYDRAZINE
DMP	DIMETHYLPOLYSILOXANE
DMS	DIMETHYL SULFOXIDE
DMT	DIMETHYL TEREPHTHALATE
DMZ	DIMETHYLZINC
DNA	DI-n-PROPYLAMINE
DNB	m-DINITROBENZENE
DNC	DINITROCRESOLS
DNP	2,4-DINITROPHENOL
DNT	2,4-DINITROANILINE
DOA	DIOCTYL ADIPATE
DOD	DODECENE
DOP	DIOCTYL PHTHALATE
DOX	1,4-DIOXANE
DPA	DIBUTYL PHTHALATE
DPD	DIPHENYLDICHLOROSILANE
DPE	DIPHENYL ETHER
DPG	DIPROPYLENE GLYCOL
DPH	DIETHYL PHTHALATE
DPM	DIPHENYLMETHANE DIISOCYANATE

TABLE A-1. INDEX OF CODES (CONTINUED)

DPM	DIPENTENE
DPO	DIBENZOYL PEROXIDE
DPP	DICHLOROPROPANE
DPR	DICHLOROPROPENE
DPT	DICYCLOPENTADIENE
DSD	DODECYL SULFATE, DIETHANOLAMINE SALT
DSF	DIMETHYL SULFATE
DSL	DIMETHYL SULFIDE
DSM	DODECYL SULFATE, MAGNESIUM SALT
DSR	DISTILLATES: STRAIGHT RUN
DSS	DIOCTYL SODIUM SULFOSUCCINATE
DST	DODECYL SULFATE, TRIETHANOLAMINE SALT
DTC	DODECYLTRICHLOROSILANE
DTH	DOWTHERM
DTM	4,4'-DICHLORO-alpha-TRICHLOROMETHYL-BENZHYDROL
DTN	DEMETON
DTS	DEXTROSE SOLUTION
DTT	2,4-DINITROTOLUENE
DZN	DIAZINON
DZP	DI-(p-CHLOROBENZOYL) PEROXIDE
EAA	ETHYL ACETOACETATE
EAC	ETHYL ACRYLATE
EAD	ETHYLALUMINUM DICHLORIDE
EAI	2-ETHYLHEXYL ACRYLATE, INHIBITED
EAL	ETHYL ALCOHOL
EAM	ETHYLAMINE
EAS	ETHYLALUMINUM SESQUICHLORIDE
EBR	ETHYL BUTYRATE
EBT	ETHYL BUTANOL
ECA	ETHYL CHLOROACETATE
ECF	ETHYL CHLOROFORMATE
ECH	ETHYLENE CHLOROHYDRIN
ECL	ETHYL CHLORIDE

TABLE A-1. INDEX OF CODES (CONTINUED)

ECS	ETHYLDICHLOROSILANE
EDA	ETHYLENEDIAMINE
EDB	ETHYLENE BIBROMIDE
EDC	ETHYLENE DICHLORIDE
EDR	ENDRIN
EDT	ETHYLENEDIAMINE TETRACETIC ACID
EEE	ETHYLENE GLYCOL DIETHYL ETHER
EET	ETHYL ETHER
EFM	ETHYL FORMATE
EGA	ETHYLENE GLYCOL MONOETHYL ETHER ACETATE
EGD	ETHYLENE GLYCOL DIMETHYL ETHER
EGE	ETHYLENE GLYCOL MONOETHYL ETHER
EGL	ETHYLENE GLYCOL
EGM	ETHYLENE GLYCOL MONOBUTYL ETHER
EGY	ETHYLENE GLYCOL DIACETATE
EHA	ETHYLHEXALDEHYDE
EHP	ETHOXYDIHYDROPYRAN
EHT	ETHYL HEXYL TALLATE
EHX	2-ETHYL HEXANOL
ELT	ETHYL LACTATE
EMA	ETHYLENE GLYCOL MONOBUTYL ETHER ACETATE
EMC	ETHYL MERCAPTAN
EME	ETHYLENE GLYCOL MONOMETHYL ETHER
ENB	ETHYLIDENENORBORNENE
ENP	ETHOXYLATED NONYLPHENOL
EOD	ETHOXYLATED DODECANOL
EOP	ETHOXYLATED PENTADECANOL
EOT	ETHOXYLATED TETRADECANOL
EOX	ETHYLENE OXIDE
EPA	2-ETHYL-3-PROPYLACROLEIN
EPC	EPICHLOROHYDRIN
EPD	ETHYL PHOSPHONOTHIOIC DICHLORIDE, ANHYDROUS
EPP	ETHYL PHOSPHORODICHLORIDATE
EPS	ETHYLPHENYLDICHLOROSILANE

TABLE A-1. INDEX OF CODES (CONTINUED)

ESC	ETHYL SILICATE
ETA	ETHYL ACETATE
ETB	ETHYLBENZENE
ETC	ETHYLENE CYANOHYDRIN
ETD	ETHOXYLATED TRIDECANOL
ETG	ETHOXY TRIGLYCOL
ETH	ETHANE
ETI	ETHYLENEIMINE
ETL	ETHYLENE
ETM	ETHYL METHACRYLATE
ETN	ETHYL NITRITE
ETS	ETHYLTRICHLOROSILANE
EVO	EPOXIDIZED VEGETABLE OILS
FAC	FERRIC AMMONIUM CITRATE
FAL	FURFURYL ALCOHOL
FAO	FERRIC AMMONIUM OXALATE
FAS	FERROUS AMMONIUM SULFATE
FCL	FERRIC CHLORIDE
FCP	FERRIC GLYCEROPHOSPHATE
FEC	FERROUS CHLORIDE
FFA	FURFURAL
FFB	FERROUS FLUOROBORATE
FMA	FORMIC ACID
FMS	FORMALDEHYDE SOLUTION
FNT	FERRIC NITRATE
FOX	FERROUS OXALATE
FRS	FERROUS SULFATE
FSA	FLUOSULFONIC ACID
FSF	FERRIC SULFATE
FSL	FLUOSILICIC ACID
FUM	FUMARIC ACID
FXX	FLUORINE

TABLE A-1. INDEX OF CODES (CONTINUED)

GAK	GASOLINE BLENDING STOCKS: ALKYLATES
GAT	GASOLINES: AUTOMOTIVE (< 4.23g LEAD/GAL.)
GAV	GASOLINES: AVIATION (< 4.86g LEAD/GAL.)
GCM	GLYCIDYL METHACRYLATE
GCR	GLYCERINE
GCS	GASOLINES: CASINGHEAD
GLA	GALLIC ACID
GOC	GAS OIL: CRACKED
GOS	GLYOXAL, 40% SOLUTION
GPL	GASOLINES: POLYMER
GRF	GASOLINE BLENDING STOCKS: REFORMATES
GSR	GASOLINES: STRAIGHT RUN
GTA	GLUTARALDEHYDE SOLUTION
HAC	HEXADECYLTRIMETHYLAMMONIUM CHLORIDE
HAI	2-HYDROXYETHYL ACRYLATE, INHIBITED
HAL	n-HEXALDEHYDE
HAS	HYDROXYLAMINE SULFATE
HBR	HYDROGEN BROMIDE
HCC	HEXACHLOROCYLOPENTADIENE
HCL	HYDROCHLORIC ACID
HCN	HYDROGEN CYANIDE
HDC	HYDROGEN CHLORIDE
HDQ	HYDROQUINONE
HDS	HYDROGEN SULFIDE
HDZ	HYDRAZINE
HFA	HYDROFLUORIC ACID
HFX	HYDROGEN FLUORIDE
HMD	HEXAMETHYLENEDIAMINE
HMI	HEXAMETHYLENEIMINE
HMT	HEXAMETHYLENETETRAMINE
HPA	HYDROXYPROPYL ACRYLATE
HPM	HYDROXYPROPYL METHACRYLATE

TABLE A-1. INDEX OF CODES (CONTINUED)

HPO	HYDROGEN PEROXIDE
HPT	HEPTANE
HSS	HEXADECYL SULFATE, SODIUM SALT
HTC	HEPTACHLOR
HTE	1-HEPTENE
HTN	HEPTANOL
HXA	HEXANE
HXE	1-HEXENE
HXG	HEXYLENE GLYCOL
HXN	HEXANOL
HXX	HYDROGEN, LIQUEFIED
IAA	ISOAMYL ALCOHOL
IAC	ISOPROPYL ACETATE
IAI	ISODECYL ACRYLATE, INHIBITED
IAL	ISOBUTYL ALCOHOL
IAM	ISOBUTYLAMINE
IBA	ISOBUTYL ACETATE
IBL	ISOBUTYLENE
IBN	ISOBUTYRONITRILE
IBR	ISOBUTYRIC ACID
IBT	ISOBUTANE
IDA	ISODECALDEHYDE
IHA	ISOHEXANE
IOA	ISOOCTYL ALCOHOL
IOC	ISOOCTALDEHYDE
IPA	ISOPROPYL ALCOHOL
IPC	ISOPROPYL PERCARBONATE
IPE	ISOPROPYL ETHER
IPH	ISOPHORONE
IPL	ISOPHTHALIC ACID
IPM	ISOPROPYL MERCAPTAN
IPP	ISOPROPYLAMINE
IPR	ISOPRENE
IPT	ISOPENTANE

TABLE A-1. INDEX OF CODES (CONTINUED)

ISA	ISODECYL ALCOHOL
IVA	ISOVALERALDEHYDE
JPF	JET FUELS: JP-4
JPO	JET FUELS: JP-1 (KEROSENE)
JPT	JET FUELS: JP-3
JPV	JET FUELS: JP-5 (KEROSENE, HEAVY)
KRS	KEROSENE
LAC	LEAD ACETATE
LAH	LITHIUM ALUMINUM HYDRIDE
LAL	LINEAR ALCOHOLS (12-15 CARBON)
LAR	LEAD ARSENATE
LFB	LEAD FLUOROBORATE
LFR	LEAD FLUORIDE
LHD	LITHIUM HYDRIDE
LID	LEAD IODIDE
LLS	LATEX, LIQUID SYNTHETIC
LNG	LIQUEFIED NATURAL GAS
LNT	LEAD NITRATE
LPG	LIQUEFIED PETROLEUM GAS
LPO	LAUROYL PEROXIDE
LRM	LAURYL MERCAPTAN
LTA	LACTIC ACID
LTC	LEAD THIOCYANATE
LTH	LITHARGE
LTM	LITHIUM, METALLIC
LTT	LEAD TETRAACETATE
MAA	METHYL AMYL ALCOHOL
MAC	METHYL AMYL ACETATE
MAL	METHYL ALCOHOL
MAM	METHYL ACRYLATE

TABLE A-1. INDEX OF CODES (CONTINUED)

MAN	N-METHYLANILINE
MAP	METHYL ACETYLENE - PROPADIENE MIXTURE
MAT	MERCURIC ACETATE
MBK	METHYL n-BUTYL KETONE
MCA	MONOCHLOROACETIC ACID
MCC	MERCURIC AMMONIUM CHLORIDE
MCF	MONOCHLORODIFLUOROMETHANE
MCH	METHYL CHLOROFORMATE
MCL	METHALLYL CHLORIDE
MCN	MERCURIC CYANIDE
MCP	METHYLCYCLOPENTANE
MCR	MERCURY
MCS	METHYLDICHLOROSILANE
MCT	METHYLCYCLOPENTADIENYLMANGANESE TRICARBONYL
MEA	MONOETHANOLAMINE
MEK	METHYL ETHYL KETONE
MEP	METHYLETHYLPYRIDINE
MFA	MOTOR FUEL ANTI-KNOCK COMPOUNDS CONTAINING LEAD ALKYLS
MFM	METHYL FORMATE
MGX	MAGNESIUM
MHZ	METHYLHYDRAZINE
MIC	METHYL ISOBUTYL CARBINOL
MID	MERCURIC IODIDE
MIK	METHYL ISOBUTYL KETONE
MLA	MALEIC ANHYDRIDE
MLH	MALEIC HYDRAZIDE
MLI	MALEIC ACID
MLT	MALATHION
MMC	METHYL MERCAPTAN
MMM	METHYL METHACRYLATE
MNS	MINERAL SPIRITS
MNT	MERCURIC NITRATE
MOC	METHOXYCHLOR

TABLE A-1. INDEX OF CODES (CONTINUED)

MOX	MERCURIC OXIDE
MPA	MONOISOPROPANOLAMINE
MPC	MAGNESIUM PERCHLORATE
MPD	METHYL PHOSPHONOTHIOIC DICHLORIDE (ANHYD)
MPK	METHYL ISOPROPENYL KETONE, INHIBITED
MPL	MORPHOLINE
MPT	METHYL PARATHION
MPY	1-METHYLPYRROLIDONE
MRC	MERCURIC CHLORIDE
MRN	MERCUROUS NITRATE
MRR	MERCUROUS CHLORIDE
MSA	METHANEARSONIC ACID, SODIUM SALTS
MSF	MERCURIC SULFIDE
MSO	MESITYL OXIDE
MSR	alpha-METHYLSTYRENE
MTA	METHYLAMINE
MTB	METHYL BROMIDE
MTC	METHYL CHLORIDE
MTF	METHYL FORMAL
MTH	METHANE
MTO	MOLYBDIC TRIOXIDE
MTS	METHYLTRICHLOROSILANE
MTT	METHYL ACETATE
MVK	METHYL VINYL KETONE
NAA	NITRILOTRIACETIC ACID AND SALTS
NAB	NABAM
NAC	NITRIC ACID
NAL	4-NITROANILINE
NAN	NONANE
NAO	1-NAPHTHYLAMINE
NAS	NICKEL AMMONIUM SULFATE
NBR	NICKEL BROMIDE
NCL	NICKEL CHLORIDE

TABLE A-1. INDEX OF CODES (CONTINUED)

NCN	NICKEL CYANIDE
NCS	NICOTINE SULFATE
NC1	NAPHTHA: COAL TAR
NFB	NICKEL FLUOROBORATE
NFM	NICKEL FORMATE
NHX	NEOHEXANE
NIC	NICOTINE
NKA	NICKEL ACETATE
NKC	NICKEL CARBONYL
NKS	NICKEL SULFATE
NMT	NITROMETHANE
NNE	1-NONENE
NNN	NONANOL
NNP	NONYLPHENOL
NNT	NICKEL NITRATE
NON	NONENE
NOX	NITROGEN TETROXIDE
NPH	4-NITROPHENOL
NPP	2-NITROPROPANE
NSS	NAPHTHA: STODDARD SOLVENT
NSV	NAPHTHA: SOLVENT
NTA	2-NITROANILINE
NTB	NITROBENZENE
NTC	NITROSYL CHLORIDE
NTE	NITROETHANE
NTI	NAPTHENIC ACIDS
NTL	NITRALIN
NTM	NAPHTHALENE, MOLTEN
NTO	NITROUS OXIDE
NTP	2-NITROPHENOL
NTX	NITRIC OXIDE
NVM	NAPHTHA: VM & P (75% NAPHTHA)
NXX	NITROGEN, LIQUEFIED

TABLE A-1. INDEX OF CODES (CONTINUED)

OAC	OLEIC ACID, SODIUM SALT
OAN	OCTANE
OAP	OLEIC ACID, POTASSIUM SALT
OAS	OILS, MISCELLANEOUS: ABSORPTION
OCA	OILS, EDIBLE: CASTOR
OCC	OILS, EDIBLE: COCONUT
OCF	OILS: CLARIFIED
OCR	OILS, MISCELLANEOUS: CROTON
OCS	OILS, EDIBLE: COTTONSEED
OCT	OILS, MISCELLANEOUS: COAL TAR
ODS	OILS: DIESEL
OET	OCTYL EPOXY TALLATE
OFR	OILS, FUEL: NO. 4
OFS	OILS, EDIBLE: FISH
OFV	OILS, FUEL: NO. 5
OIL	OILS: CRUDE
OLA	OLEIC ACID
OLB	OILS, MISCELLANEOUS: LUBRICATING
OLD	OILS, EDIBLE: LARD
OLM	OLEUM
OLS	OILS, MISCELLANEOUS: LINSEED
OMN	OILS, MISCELLANEOUS: MINERAL
OMS	OILS, MISCELLANEOUS: MINERAL SEAL
OMT	OILS, MISCELLANEOUS: MOTOR
ONF	OILS, MISCELLANEOUS: NEATSFOOT
OOD	OILS, FUEL: NO. 1-D
OOL	OILS, EDIBLE: OLIVE
OON	OILS, FUEL: NO. 1 (KEROSENE)
OPM	OILS, EDIBLE: PALM
OPN	OILS, EDIBLE: PEANUT
OPT	OILS, MISCELLANEOUS: PENETRATING
ORD	OILS, MISCELLANEOUS: ROAD
ORG	OILS, MISCELLANEOUS: RANGE

TABLE A-1. INDEX OF CODES (CONTINUED)

ORN	OILS, MISCELLANEOUS: ROSIN
ORS	OILS, MISCELLANEOUS: RESIN
OSB	OILS, EDIBLE: SOYA BEAN
OSD	OILS, MISCELLANEOUS: SPINDLE
OSF	OILS, EDIBLE: SAFFLOWER
OSP	OILS, MISCELLANEOUS: SPERM
OSX	OILS, FUEL: NO. 6
OSY	OILS, MISCELLANEOUS: SPRAY
OTA	OCTANOL
OTB	OILS, MISCELLANEOUS: TURBINE
OTC	OILS, EDIBLE: TUCUM
OTD	OILS, FUEL: NO. 2-D
OTE	1-OCTENE
OTF	OILS, MISCELLANEOUS: TRANSFORMER
OTL	OILS, MISCELLANEOUS: TALL
OTN	OILS, MISCELLANEOUS: TANNER'S
OTW	OILS, FUEL: NO. 2
OVG	OILS, EDIBLE: VEGETABLE
OXA	OXALIC ACID
OXY	OXYGEN, LIQUEFIED
PAA	PERACETIC ACID
PAC	PHOSPHORIC ACID
PAD	PROPIONALDEHYDE
PAH	PROPIONIC ANHYDRIDE
PAL	n-PROPYL ALCOHOL
PAN	PHTHALIC ANHYDRIDE
PAS	POTASSIUM ARSENATE
PAT	n-PROPYL ACETATE
PBO	POTASSIUM BINOXALATE
PBP	PROPYLENE BUTYLENE POLYMER
PBR	PHOSPHORUS TRIBROMIDE
PCB	POLYCHLORINATED BIPHENYL
PCH	POTASSIUM CHROMATE
PCL	PERCHLORIC ACID

TABLE A-1. INDEX OF CODES (CONTINUED)

PCM	PERCHLOROMETHYL MERCAPTAN
PCP	PENTACHLOROPHENOL
PCR	POTASSIUM CHLORATE
PDC	PENTADECANOL
PDL	PHENYLDICHLOROARSINE, LIQUID
PDT	POTASSIUM DICHLORO-s-TRIAZINETRIONE
PET	PENTAERYTHRITOL
PFA	PARAFORMALDEHYDE
PGA	PYROGALLIC ACID
PGC	POLYPROPYLENE GLYCOL
PGM	POLYPROPYLENE GLYCOL METHYL ETHER
PHG	PHOSGENE
PHH	PHENYLHYDRAZINE HYDROCHLORIDE
PHN	PHENOL
PII	PROPYLENEIMINE, INHIBITED
PLB	POLYBUTENE
PLP	POLYPROPYLENE
PLT	beta-PROPIOLACTONE
PME	PROPYLENE GLYCOL METHYL ETHER
PMM	n-PROPYL MERCAPTAN
PNA	PROPIONIC ACID
POP	POTASSIUM PEROXIDE
POX	PROPYLENE OXIDE
PPA	POLYPHOSPHORIC ACID
PPG	PROPYLENE GLYCOL
PPI	POLYMETHYLENE POLYPHENYL ISOCYANATE
PPL	PROPYLENE
PPO	PHOSPHORUS OXYCHLORIDE
PPP	PHOSPHORUS PENTASULFIDE
PPR	PHOSPHORUS, RED
PPT	PHOSPHORUS TRICHLORIDE
PPW	PHOSPHORUS, WHITE
PPZ	PIPERAZINE
PRD	PYRIDINE
PRP	PROPANE

TABLE A-1. INDEX OF CODES (CONTINUED)

PTA	PENTANE
PTB	PENTABORANE
PTC	POTASSIUM CYANIDE
PTD	POTASSIUM DICHROMATE
PTE	1-PENTENE
PTH	POTASSIUM HYDROXIDE
PTI	POTASSIUM IODIDE
PTL	PETROLATUM
PTM	POTASSIUM, METALLIC
PTN	PETROLEUM NAPHTHA
PTO	PARATHION, LIQUID
PTP	POTASSIUM PERMANGANATE
PTS	POTASSIUM OXALATE
PTT	PROPYLENE TETRAMER
QNL	QUINOLINE
RSC	RESORCINOL
SAB	SODIUM ALKYLBENZENESULFONATES
SAC	SULFURIC ACID, SPENT
SAM	SODIUM AMIDE
SAR	SODIUM ARSENITE
SAS	SODIUM ALKYL SULFATES
SAZ	SODIUM AZIDE
SBH	SODIUM BOROHYDRIDE
SBS	SODIUM BISULFITE
SBT	SORBITOL
SCD	SODIUM CACODYLATE
SCH	SODIUM CHROMATE
SCL	SULFURYL CHLORIDE
SCN	SODIUM CYANIDE
SCR	SODIUM DICHROMATE
SCY	SODIUM THIOCYANATE

TABLE A-1. INDEX OF CODES (CONTINUED)

SDA	SODIUM ARSENATE
SDB	SODIUM BORATE
SDC	SODIUM CHLORATE
SDF	SODIUM FLUORIDE
SDH	SODIUM HYDRIDE
SDS	SODIUM SULFIDE
SDT	SODIUM DICHLORO-s-TRIAZINETRIONE
SDU	SODIUM
SFA	SULFURIC ACID
SFC	SODIUM FERROCYANIDE
SFD	SULFUR DIOXIDE
SFL	SULFOLANE
SFM	SULFUR MONOCHLORIDE
SFR	SODIUM SILICOFLUORIDE
SHC	SODIUM HYPOCHLORITE
SHD	SODIUM HYDROXIDE
SHS	SODIUM HYDROSULFIDE SOLUTION
SLA	SALICYLIC ACID
SLD	SELENIUM DIOXIDE
SML	SODIUM METHYLATE
SNT	SODIUM NITRITE
SOX	SODIUM OXALATE
SPP	SODIUM PHOSPHATE
SRA	STEARIC ACID
SRS	SUCROSE
SSC	SODIUM SILICATE
SSF	SODIUM SULFITE
STC	SILICON TETRACHLORIDE
STO	SELENIUM TRIOXIDE
STY	STYRENE
SVA	SILVER ACETATE
SVC	SILVER CARBONATE
SVF	SILVER FLUORIDE
SVI	SILVER IODATE

TABLE A-1. INDEX OF CODES (CONTINUED)

SVN	SILVER NITRATE
SVO	SILVER OXIDE
SVS	SILVER SULFATE
SXX	SULFUR (LIQUID)
TAL	TRIETHYLALUMINUM
TAP	p-TOLUENESULFONIC ACID
TBT	TETRABUTYL TITANATE
TCA	2,4,5-TRICHLOROPHENOXYACETIC ACID
TCE	TRICHLOROETHANE
TCF	TRICHLOROFLUOROMETHANE
TCL	TRICHLOROETHYLENE
TCP	TRICRESYL PHOSPHATE
TCS	TRICHLOROSILANE
TCT	TRICHLORO-s-TRIAZINETRIONE
TDB	TETRADECYLBENZENE
TDC	1-TRIDECENE
TDI	TOLUENE 2,4-DIISOCYANATE
TDN	TRIDECANOL
TEA	TRIETHANOLAMINE
TEB	TRIETHYLBENZENE
TEC	TETRACHLOROETHANE
TED	TETRAETHYL DITHIOPYROPHOSPHATE
TEG	TRIETHYLENE GLYCOL
TEL	TETRAETHYL LEAD
TEN	TRIETHYLAMINE
TEP	TETRAETHYL PYROPHOSPHATE
TES	2,4,5-T (ESTERS)
TET	TRIETHYLENETETRAMINE
TFA	TALLOW FATTY ALCOHOL
TFC	TRIFLUOROCHLOROETHYLENE
TFE	TETRAFLUOROETHYLENE, INHIBITED
TFR	TRIFLURALIN
TGC	TRIPROPYLENE GLYCOL
THF	TETRAHYDROFURAN

TABLE A-1. INDEX OF CODES (CONTINUED)

THN	TETRAHYDRONAPHTHALENE
THR	THIRAM
TIA	TRIISOBUTYLALUMINUM
TLI	o-TOLUIDINE
TLO	TALLOW
TMA	TRIMETHYLAMINE
TMC	TRIMETHYLCHLOROSILANE
TML	TETRAMETHYL LEAD
TNA	TANNIC ACID
TOL	TOLUENE
TPG	THIOPHOSGENE
TPH	TRICHLOROPHENOL
TPO	TRIS(AZIRIDINYL)PHOSPHINE OXIDE
TPT	TURPENTINE
TRN	THORIUM NITRATE
TTD	1-TETRADECENE
TTE	TETRACHLOROETHYLENE
TTG	TETRAETHYLENE GLYCOL
TTN	TETRADECANOL
TTP	TETRAETHYLENEPENTAMINE
TTT	TITANIUM TETRACHLORIDE
TXP	TOXAPHENE
UAN	URANYL NITRATE
UDB	n-UNDECYLBENZENE
UDC	1-UNDECENE
UND	UNDECANOL
UPO	UREA PEROXIDE
URA	URANYL ACETATE
URE	UREA
URS	URANYL SULFATE
VAL	VALERALDEHYDE
VAM	VINYL ACETATE

TABLE A-1. INDEX OF CODES (CONCLUDED)

VCI	VINYLIDENECHLORIDE, INHIBITED
VCM	VINYL CHLORIDE
VFI	VINYL FLUORIDE, INHIBITED
VME	VINYL METHYL ETHER, INHIBITED
VMT	VINYLTOLUENE
VOT	VANADIUM OXYTRICHLORIDE
VOX	VANADIUM PENTOXIDE
VSF	VANADYL SULFATE
VTS	VINYLTRICHLOROSILANE
WCA	WAXES: CARNAUBA
WPF	WAXES: PARAFFIN
XLM	m-XYLENE
XLO	o-XYLENE
XLP	p-XYLENE
XYL	XYLENOL
ZAC	ZINC AMMONIUM CHLORIDE
ZAR	ZINC ARSENATE
ZBO	ZINC BORATE
ZBR	ZINC BROMIDE
ZCA	ZIRCONIUM ACETATE
ZCL	ZINC CHLORIDE
ZCO	ZIRCONIUM OXYCHLORIDE
ZCR	ZINC CHROMATE
ZCS	ZIRCONIUM SULFATE
ZDP	ZINC DIALKYLDITHIOPHOSPHATE
ZFB	ZINC FLUOROBORATE
ZIR	ZIRCONIUM NITRATE
ZNA	ZINC ACETATE
ZNT	ZINC NITRATE
ZPP	ZINC PHOSPHIDE
ZPS	ZINC PHENOLSULFONATE
ZSP	ZINC SULFATE
ZSL	ZINC SILICOFLUORIDE

APPENDIX B

SELECTED SYNONYMS

This appendix lists the synonyms, in alphabetical order, for a selected group of chemical compounds listed in Appendix A (see Table B-1). For each synonym listed in the left-hand column, the corresponding name of the chemical is given in the right-hand column. Chemical names are also listed as synonyms to give a master list of names for these chemicals.

TABLE B-1. SELECTED SYNONYMS

SYNONYM		COMPOUND NAME
Acetic acid, ethyl ester	=	Ethyl acetate
Acetic ester	=	Ethyl acetate
Acetic ether	=	Ethyl acetate
Alcohol	=	Ethyl alcohol
Algylen	=	Trichloroethylene
Arochlor	=	Polychlorinated biphenyl (PCB)
Benzene	=	Benzene
1,4-Benzenediol	=	Hydroquinone
1,2,3-Benzenetriol	=	Pyrogallic acid
Benzol	=	Benzene
Benzole	=	Benzene
s-(1,2-Bis(ethoxycarbonyl)ethyl)-O,O-dimethyl phosphorodithioate	=	Malathion
Carbamide	=	Urea
Carbinol	=	Methyl alcohol
Carbonyldiamide	=	Urea
Chlorinated biphenyl	=	Polychlorinated biphenyl (PCB)
Chlorylen	=	Trichloroethylene
Cologne spirit	=	Ethyl alcohol

TABLE B-1. SELECTED SYNONYMS (CONTINUED)

SYNONYM		COMPOUND NAME
Colonial spirit	=	Methyl alcohol
Columbian spirit	=	Methyl alcohol
Cresols	=	Cresols
Cresylic acids	=	Cresols
CYTHION insecticide	=	Malathion
Denatured alcohol	=	Ethyl alcohol
s-(1,2-Dicarbethoxyethyl)-O,O-dimethyl dithiophosphate	=	Malathion
Dichloromethane	=	Dichloromethane
p-Dihydroxybenzene	=	Hydroquinone
1,2-Dihydroxyethane	=	Ethylene glycol
Dimazine	=	1,1-Dimethylhydrazine
1,1-Dimethylhydrazine	=	1,1-Dimethylhydrazine
unsym-Dimethylhydrazine	=	1,1-Dimethylhydrazine
Drycleaners naphtha	=	Naphtha:stoddard solvent
1,2-Ethanediol	=	Ethylene glycol
Ethanol	=	Ethyl alcohol
Ethyl acetate	=	Ethyl acetate
Ethyl alcohol	=	Ethyl alcohol

TABLE B-1. SELECTED SYNONYMS (CONTINUED)

SYNONYM		COMPOUND NAME
Ethylene dihydrate	=	Ethylene glycol
Ethylene glycol	=	Ethylene glycol
Ethyl ethanoate	=	Ethyl acetate
Fermentation alcohol	=	Ethyl alcohol
Gasoline, automotive (less than 4.23 g lead/gal)	=	Gasoline, automotive (less than 4.23 g lead/gal)
Gasoline, aviation (less than 4.86 g lead/gal)	=	Gasoline, aviation (less than 4.86 g lead/gal)
Gasoline blending stocks:alkylates	=	Gasoline blending stocks:alkylates
Gasoline blending stocks:reformates	=	Gasoline blending stocks:reformates
Gasoline:casinghead	=	Gasoline:casinghead
Gasoline:polymer	=	Gasoline:polymer
Gasoline:straight run	=	Gasoline:straight run
Glycol	=	Ethylene glycol
Grain alcohol	=	Ethyl alcohol
Gremalgene	=	Trichloroethylene
Halogenated waxes	=	Polychlorinated biphenyl (PCB)
Hydrazine	=	Hydrazine
Hydroquinol	=	Hydroquinone

TABLE B-1. SELECTED SYNONYMS (CONTINUED)

SYNONYM		COMPOUND NAME
Hydroquinone	=	Hydroquinone
Hydroxytoluenes	=	Cresols
Jet fuel:JP-4	=	Jet fuel:JP-4
Liquid petrolatum	=	Oil:mineral
Malathion	=	Malathion
Mercaptosuccinic acid, s-ester with O,O-dimethyl dithiophosphate	=	Malathion
Methanol	=	Methyl alcohol
Methyl alcohol	=	Methyl alcohol
Methylbenzene	=	Toluene
Methylbenzol	=	Toluene
Methylene chloride	=	Dichloromethane
Methylene dichloride	=	Dichloromethane
Methylhydrazine	=	Methylhydrazine
Methylphenols	=	Cresols
Mineral oil	=	Oil:mineral
MMH	=	Methylhydrazine
Monoethylene glycol	=	Ethylene glycol
Monomethylhydrazine	=	Methylhydrazine

TABLE B-1. SELECTED SYNONYMS (CONTINUED)

SYNONYM		COMPOUND NAME
Motor spirit	=	Gasoline, automotive (less than 4.23 g lead/gal)
Naphtha:stoddard solvent	=	Naphtha:stoddard solvent
Natural gasoline	=	Gasoline:casinghead
Oil:mineral	=	Oil:mineral
Oxytoluenes	=	Cresols
PCB	=	Polychlorinated biphenyl (PCB)
Petrol	=	Gasoline, automotive (less than 4.23 g lead gal)
Petroleum solvent	=	Naphtha:stoddard solvent
Polychlorinated biphenyl (PCB)	=	Polychlorinated biphenyl (PCB)
Polychloropolyphenyls	=	Polychlorinated biphenyl (PCB)
Pyrogallic acid	=	Pyrogallic acid
Pyrogallol	=	Pyrogallic acid
Pyrogentisic acid	=	Hydroquinone
Pyroxylic spirit	=	Methyl alcohol
Quinol	=	Hydroquinone
Spirit	=	Ethyl alcohol
Spirits of wine	=	Ethyl alcohol

TABLE B-1. SELECTED SYNONYMS (CONTINUED)

SYNONYM		COMPOUND NAME
Spotting naphtha	=	Naphtha:stoddard solvent
Streunex	=	Benzene
Tar acids	=	Cresols
Threthylene	=	Trichloroethylene
Toluene	=	Toluene
Toluol	=	Toluene
Trethylene	=	Trichloroethylene
Tri	=	Trichloroethylene
Trichloran	=	Trichloroethylene
Trichloroethene	=	Trichloroethylene
Trichloroethylene	=	Trichloroethylene
Triclene	=	Trichloroethylene
Tri-Clene	=	Trichloroethylene
Trielene	=	Trichloroethylene
1,2,3-Trihydroxybenzene	=	Pyrogallic acid
Trilene	=	Trichloroethylene
Triline	=	Trichloroethylene
Trimar	=	Trichloroethylene
UDMH	=	1,1-Dimethylhydrazine

TABLE B-1. SELECTED SYNONYMS (CONCLUDED)

SYNONYM		COMPOUND NAME
Urea	=	Urea
White oil	=	Oil:mineral
Wood alcohol	=	Methyl alcohol
Wood naphtha	=	Methyl alcohol
Wood spirit	=	Methyl alcohol

APPENDIX C

HACS SYSTEM AND ERROR MESSAGES

Given below are identifications and descriptions of general diagnostic and informative messages incorporated in the overall HACS structure for user input data processing, state file interactions, assessment model sequencing, and output data production. The messages included in this section apply to the interim interactive version of the system and thus are a subset of the full group of messages. Additional messages, specific to the normal interactive user dialog, are described in the text of the manual.

HACS messages described below are given in both normal and abnormal processing. Most error conditions or warning messages for potential errors are denoted by a string of five asterisks printed at the start of the message. Where appropriate, each message below indicates using lower case letters to type specific information included by HACS under program control, depending on the conditions under which the message is generated.

AN ERROR WAS MADE IN READING THE DATA BASE -- MODEL code. EXECUTION OF MODEL code IS TERMINATED.

The message, given with the appropriate rate model designation inserted, indicates that, during the transfer of field data values from the state file for input to the requested rate model, at least one and possibly more errors were encountered. This condition is completely program controlled, and an error in the user input data is not indicated. The sequence of model input operations is explicitly defined by the program code written for each

rate model, and the error condition indicates either an incorrect modification of the program code, or that a field required by a rate model has not been defined in the HACS default file.

Specifically, this condition will occur if a rate model attempts to use a field for which the field number has not been entered in the default file, or if the rate model code requests a type of value (real or integer) which is inconsistent with the type of value (real or integer) of the field entered in the default file. All remaining model operations which would otherwise normally be performed are terminated; HACS will however continue to attempt to execute the next model requested.

COMPUTATION OF FUNCTIONS OF TEMPERATURE FOLLOW USING TEMPERATURES OF ...

This message precedes a display of the ambient and boiling temperatures that are used in computations of functions of temperature during the transfer of chemical data from the property file to the HACS state file.

COMPUTATION OF identification ...

A header message used to indicate HACS is computing values of the identified function of temperature at both ambient and boiling temperatures. Messages following indicate values obtained as well as any abnormal conditions.

COMPUTATION USES TEMPERATURE AT LIMIT OF RANGE

Additional message, following warning condition, indicates that a chemical property function of temperature is being computed at an overriding range limit and not at the value of ambient or boiling temperature specified.

END OF HACS RUN

Message is written by HACS on printed output to indicate completion of user requested operations. May be given either on completion of all user requests or on abnormal conditions causing program controlled premature termination of processing.

*****ERROR - COMPUTATION OF FUNCTION VALUE UNABLE TO PROCEED

A data base recall error occurred during the collection of temperature function coefficients. This error is caused by program inconsistencies in calls to subroutine COEF and is not a user error.

*****ERROR*****DIVIDE FAULT OCCURRED DURING EXECUTION OF OVERLAY n

*****ERROR*****EXPONENT OVERFLOW OCCURRED DURING EXECUTION OF OVERLAY n

*****ERROR*****ARITHMETIC FAULT OCCURRED DURING EXECUTION OF OVERLAY n

Following completion of the execution of any program overlay, HACS uses a number of system routines to test for the possible occurrence of an arithmetic fault condition and may issue one or more of the above messages with the identification of the appropriate overlay inserted. (Functionally, HACS program overlay definitions are based on groupings of rate model programs.) Generally, diagnostic conditions of this type are traced to user input inconsistent with model assumptions or limitations.

*****ERROR - FIELD NUMBER n REQUESTED FOR RECALL HAS NOT BEEN DEFINED

*****ERROR - FIELD NUMBER n REQUESTED FOR SAVE HAS NOT BEEN DEFINED

An operation to recall (or save) a data value from (in) the HACS state file has requested a value for a field number (inserted in the message) which is undefined. Either a program modification has been made to a rate model using an incorrect field number, or the definition of the field is

missing from the HACS default file.

*****ERROR - REAL RECALL REQUESTED FOR INTEGER FIELD number name

*****ERROR - REAL SAVE REQUESTED FOR INTEGER FIELD number name

*****ERROR - INTEGER RECALL REQUESTED FOR REAL FIELD number name

*****ERROR - INTEGER SAVE REQUESTED FOR REAL FIELD number name

The use of data values in the state file is controlled by the type of program operation coded within an assessment rate model, and a data type indicator (integer, real) is included as part of the data item definition in the HACS default file. These error messages, which should not occur during normal HACS operation, indicate either an improperly coded data base operation request within a rate model, or an incorrect, or inconsistent, data-type definition in the HACS default file for the field identified in the message. Default file definitions must not be changed without considerable caution due to the use of individual data fields by multiple routines.

FUNCTION VALUE COMPUTED AT TEMPERATURE OF value DEG. C IS ...

Where value is either ambient temperature, or the boiling temperature of the compound and the message is followed by a line giving the HACS state file field number, value, etc., for the function of temperature.

HACS STATE FILE INITIALIZED WITH identifier VALUES, FILE LABEL FOLLOWS - label

Prior to processing user input data, the HACS state file is initialized as determined by previous operations during the run and the options specified by the user operations input. The identifier inserted in the message will be EMPTY, DEFAULT, USER, or COMPUTED as appropriate, followed by a listing of the label of the state file on initialization.

*****INPUT CONTAINS UNRECOGNIZABLE RATE MODEL CODE

A rate model code entered by the user is not A to Z, II, RR, or SS. Since the format of the rate model path input is matched to internal lists defining all valid path codes, users are cautioned to carefully check this input for invalid codes.

INSUFFICIENT DATA AVAILABLE - COMPUTATION USES REQUESTED TEMPERATURE

In the event a user specifies coefficients for a temperature function but default values are used for the bounds of the equation, the computation proceeds using the specified value of ambient or boiling temperature even though the apparent limits have been exceeded.

INSUFFICIENT DATA AVAILABLE TO EXECUTE MODEL code. EXECUTION OF MODEL code IS TERMINATED

This condition indicates an attempt was made during execution of a rate model to use an undefined field value (i.e., no values, not even default, existed for the requested field). All remaining model operations which would normally be performed are terminated; HACS will, however, continue to attempt to execute the next model requested. It should not be possible for this error condition to occur during normal processing; the most likely cause is an incorrect or inconsistent modification to internal HACS program code.

MODEL code IS NOW BEING EXECUTED. THE INPUTS REQUIRED FOR THIS RATE MODEL ARE ...

The message is printed with the appropriate rate model designation at the start of the execution of the requested model. The message is then

followed by a listing of all input data required by the rate model for execution, produced as each item is retrieved from the HACS state file and transferred to the rate model.

*****MODEL CODES NOT GIVEN IN CORRECT ASSESSMENT SEQUENCE

The structure and construction of the paths in the HACS assessment tree require that the rate model executions be performed in valid sequences which define an acceptable path along the tree. The same path code may not appear more than once, and the path codes which are given (except for rate models O, Z, II, RR, and SS) must appear in alphabetical order (A to Z). The exceptions (O, Z, II, RR, and SS) may be given in any order but may not appear more than once.

*****NOTE - VALUE IN STATE FILE OF value unit IS A identifier VALUE AND WAS NOT REPLACED

A data base save operation, displayed previously, was attempted, but the value to be stored did not have a higher source code than the existing value. The value shown in the above message remains unchanged in the HACS state file.

Number Name = value unit, IS A identifier VALUE

Where the elements in the message are inserted by HACS as:

Number = data item field number

Name = field name defined by entry in the default file for the corresponding field number

Value = numeric value currently associated with the field number, either being retrieved from the HACS state file for use in model computations, or being stored

in the HACS state file following completion of the model execution

Unit = label for the pre-selected unit or dimension of the value displayed. User options may be selected for displaying units in a single system, or for displaying field values in each different unit of measure for all systems. For this latter option, each different value and unit combination is displayed on additional lines

Identifier = defines the type or status code of the data value as:

MISSING

DEFAULT

ESTIMATE

CHEM PROP

COMPUTED

USER

SYSTEM

A priority value is associated with each of these types in ascending sequence in the order of the above list to govern the replacement of differnt values for the same field. For example, a user value entered for a field will override a value computed by HACS, but a second computed value will not replace a value computed previously by HACS. New values replace existing values in the state

file during model executions, only if the source code associated with the new value is higher than the source code associated with the existing value.

A minor inconsistency in the definition of the priority structure of the HACS state file arises during processing of user input data at the start of each run. These inputs are verified and then stored directly in the state file without priority screening. Thus, if more than one user value is entered for the same field, the last value appearing in the user input is the one saved.

OUTPUT CONTROL OPTIONS ARE ...

A header message preceding a display of the values selected for basic input/output control during an assessment run.

PHYSICAL PROPERTY DATA RETRIEVED FOR CHEMICAL code

This is followed by a listing of the compound name, path codes, shipping state, and late toxicity, as read from the property file. The message is displayed to give a listing of chemical property data which are not transferred to the HACS state file. It is given when the data for the specified chemical recognition code has been found, and precedes the actual transfer of data values into the HACS state file.

*****RUN TERMINATED

Error message is issued during user input processing, following a preceding error message, to indicate that the HACS run is unable to proceed due to errors in user input data.

STARTING SEARCH OF HACS FILE FOR PHYSICAL PROPERTIES OF CHEMICAL code ...

The actual chemical recognition code requested on user input is inserted in the message in place of the word code. This message is displayed at the start of a search of the property file, identified by a following display of the property file header (identification, creation date, version number, and back-up).

TEMPERATURE FUNCTION IS UNDEFINED

All coefficients for a function of temperature are either missing or are default values. Further computations to obtain a value are skipped, as the only result would also be a default value. The state file data priority structure would cause this value to be ignored.

THE EXECUTION OF MODEL code IS COMPLETED

The message is printed with the appropriate rate model designation inserted on completion of the model execution and prior to initiating the next requested model execution. The results of the model execution as indicated on the printed output will have been saved in the HACS state file for use as necessary in subsequent calculations.

THE RESULTS OF MODEL code ARE ...

This message follows the completion of the execution of a rate model (designation inserted) and precedes the display of model outputs.

TRANSFER OF EXACT OR ESTIMATED PROPERTY VALUES TO HACS STATE FILE FOLLOWS ...

All numeric field values, defined as exact or estimated values, are transferred from the chemical property file to the HACS state file, and are listed individually as entered in the state file. If a value has already been entered in the state file with a higher source code,

the property value is listed with additional messages to indicate the value is not saved. Any default or missing data existing on the property file for the compound is not transferred and is omitted on the HACS listing.

*****WARNING - CONVERSION OF INTEGER FIELD VALUES NOT APPLICABLE

Message is incorporated in the event that different unit labels are provided for the same integer fields in different systems of units. This condition should not occur with the currently installed version of HACS.

*****WARNING/ERROR - FIELD VALUE NOT IN RANGE min TO max unit

HACS inserts the actual values of min, max, and unit in the message. After conversion to internal CGS units, if necessary, all field values are compared to the nominal range limtis. During normal assessment runs, a warning condition occurs if either limit is exceeded by the user value. Values outside the nominal range are not permitted in the default file, and this condition causes a fatal error during default file load or update operations.

WARNING - MODEL code IS USING DEFAULT VALUES

If during immediately preceding transfer of data values from the HACS state file to an assessment rate model, one or more default values were transferred, this message is given at the conclusion of the entire data transfer sequence. Users are cautioned to carefully review all input data listings and to ensure the reasonableness of any default values in terms of the actual spill situation being assessed. This review may be used as a preliminary check to identify additional field data to be prepared for HACS input by the user.

*****WARNING - REQUESTED TEMPERATURE OF value IS NOT WITHIN RANGE value TO value

HACS inserts the actual numerical values in the message. This condition may occur in the transfer of chemical property data from the property file to HACS during the computation of properties which are functions of temperature. Either the ambient or boiling temperature, at which the values of the temperature function are computed, is not within the range of the function as defined on the property file. The computation of the function value proceeds using a value of temperature constrained to the appropriate limit. In addition, if the function value would otherwise have been assigned an exact source code, the source code is revised to indicate an estimated function value.

*****WARNING - VALUE OF FIELD number name REQUESTED TO BE SAVED EXCEEDS NOMINAL LIMITS OF value TO value unit SUBSEQUENT CALCULATIONS MAY NOT BE VALID

The value of the field identified is displayed previously and was found to be outside the nominal range (min, max) limits shown in the message. This is a warning condition only and is intended to serve as an indicator for user review and possible input revision. A likely source of error is the use of unintended input units or dimensions. Also, during the transfer of chemical data from the property file to HACS, all defined property data including functions of temperature are stored in the state file since distinctions as to whether any data item is actually necessary are made only during the execution of each rate model. In these cases, the message is only pertinent if the particular data item is actually used in any subsequent model computations.

APPENDIX D

DATA ITEM UNIT LABELS

HACS data unit labeling and conversions are governed by type codes associated with each of the data fields defined by the HACS default file. A total of 47 type codes are defined to reference 47 different series of unit labels and conversion factors in four systems of units (CGS, SI, ENG for English, and MXD for mixed). Due to differences in unit labels and conversion equations for similar quantities, the type code structure does not necessarily represent the actual type of physical quantity. Also, integer data, used for example to select output options, is non-dimensional, and unit conversion logic does not apply.

This appendix gives a list, with descriptions, of all unit labels which are defined in the current version of the system. If a unit label is missing on user input, the system will automatically assume input is in CGS units; these are displayed in the first position of the prompt message.

Conversions of all HACS data quantities (except for temperatures), for either input or output, are linear. All data is represented internally in CGS units, and the conversion factors give scales between the unit in the specified system and the CGS unit. All temperature fields are defined as type 6 quantities, and these conversions are performed using additional logic to add or subtract a constant which is defined as needed. In general, conversions of coefficients of temperature functions are non-linear (i.e., conversion equations involve all coefficient values), and, as a result of the HACS user input procedure for loading data items one at a time into the state file, a mechanism does not exist to collect all changed coefficient

values to apply the non-linear conversion equations. For this reason, unit labels for all coefficients are identical in each system, limiting the user in effect to entering values of temperature function coefficients in CGS units only. Note that full conversion capabilities are provided by the separate property file update and retrieval programs.

Unit label abbreviations are standardized, and if given by the user, must appear exactly as shown in Table D-1. The abbreviations used are defined in Table D-1.

TABLE D-1. DATA ITEM UNIT LABELS

Unit Label	Description
BT/FT2H	BTU per square foot-hour
BT/FTHF	BTU per foot-hour-degree Fahrenheit
BT/LB	BTU per pound
BT/LBF	BTU per pound-degree Fahrenheit
BT/LBMF	BTU per pound-mole-degree Fahrenheit
C	degrees Centigrade
CL/CM2S	calorie per square centimeter-second
CL/CMSC	calorie per centimeter-second-degree-Centigrade
CL/CMSC2	calorie per centimeter-second-°C-°C
CL/G	calorie per gram
CL/GC	calorie per gram - °C
CL/GC2	calorie per gram - °C-°C
CL/GK	calorie per gram-degree Kelvin
CL/GMC	calorie per gram mole - °C
CL/GMC2	calorie per gram mole-°C-°C
CL/GMC3	calorie per gram mole-°C-°C-°C
CL/GMC4	calorie per gram mole-°C-°C-°C-°C
CL/GMK	calorie per gram mole - °K
CM	centimeter
CM2	square centimeter
CM3	cubic centimeter
CM/S	centimeter per second

TABLE D-1. DATA ITEM UNIT LABELS (CONTINUED)

Unit Label	Description
CM2/S	square centimeters per second
CP	centipoise
D/CM	dynes per centimeter
D/CM2	dynes per square centimeter
DEG	degree (angular)
DS/CM2	dyne-seconds per square centimeter
F	degrees Fahrenheit
FT	feet
FT2	square feet
FT3	cubic feet
FT2/S	square feet per second
G	grams
GALS	gallons
G/CM2S	grams per square centimeter-second
G/CM3	grams per cubic centimeter
G/CM3C	grams per cubic centimeter - °C
G/CM3C2	grams per cubic centimeter-°C-°C
G/G	grams per gram
G/GM	grams per gram mole
G/HG	grams per 100 grams
G/HGC	grams per 100 grams - °C
G/KG	grams per kilogram

TABLE D-1. DATA ITEM UNIT LABELS (CONTINUED)

Unit Label	Description
G/S	grams per second
HR	hour
/HR	per hour
IN/MIN	inches per minute
J/KG	joules per kilogram
J/KGK	joules per kilogram - °K
J/KGMK	Joules per kilogram mole - °K
K	degrees Kelvin
KC/M2H	kilo-calories per square meter-hour
KC/MHK	kilo-calories per meter-hour-°K
KG	kilogram
KG/HKG	kilograms per 100 kilograms
KG/KG	kilograms per kilogram
KG/KGM	kilograms per kilogram mole
KG/M2S	kilograms per square meter-second
KG/M3	kilograms per cubic meter
KG/S	kilograms per second
KNOTS	knots
LB	pound
LB/FT3	pounds per cubic foot
LB/FT2S	pounds per square foot-second
LB/HLB	pounds per 100 pounds
LB/LB	pounds per pound

TABLE D-1. DATA ITEM UNIT LABELS (CONTINUED)

Unit Label	Description
LB/LBM	pounds per pound mole
LB/S	pounds per second
LB/S2	pounds per second-second
LN FCN	reserved for coefficient A of liquid viscosity equation
LOG-FCN	reserved for coefficient A of vapor pressure equation
M	meter
M2	square meter
M3	cubic meter
MI	miles
MIN	minute
/MIN	per minute
MM-HG	millimeters of mercury
MM/MIN	millimeters per minute
MN/M2	mega-newtons per square meter
MPH	miles per hour
M/S	meters per second
M2/S	square meters per second
NA	not applicable (for non-numeric quantities)
ND	non-dimensional
N/M	newtons per meter

TABLE D-1. DATA ITEM UNIT LABELS (CONCLUDED)

Unit Label	Description
N/M2	newtons per square meter
NS/M2	newtons-seconds per square meter
PERCENT	percent
PPM	parts per million
PSI	pounds per square inch
RAD	radians
S	second
/S	per second
TN	tons
TN/HR	tons per hour
W/M2	watts per square meter
W/MK	watts per meter - °K

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